13th INTERNATIONAL CHEMICAL AND BIOLOGICAL ENGINEERING CONFERENCE

ChemPor 2018

BOOK OF SHORT ABSTRACTS

October 02 - 04, 2018. Aveiro, Portugal

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This volume contains the short abstracts presented at the 13th International Chemical and Biological Engineering Conference (CHEMPOR 2018), held in Aveiro - Portugal, from the 2nd to the 4th of October, 2018.

University of Aveiro & Ordem dos Engenheiros

13th International Chemical and Biological Engineering Conference (CHEMPOR 2018)

Book of Short Abstracts

Edited by:
João Araújo Pereira Coutinho
Carlos Manuel Silva
José Pedro Salgado Aniceto
Marcelo Morais Rodrigues de Melo
Simão Pedro Cardoso

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Welcome Message

University of Aveiro and *Ordem dos Engenheiros* proudly welcome all participants to the 13th International Chemical and Biological Engineering Conference - CHEMPOR 2018. **Welcome to Aveiro!**

During three days, from October 2nd to 4th, more than 370 participants from Industry and Academia gathered at Centro Cultural e de Congressos de Aveiro to discuss recent developments and future directions in different areas of chemical engineering, materials science and engineering, biotechnology and biological engineering. CHEMPOR 2018 aims to be a forum for the debate of societal challenges related to energy, the environment, and the efficient use of natural resources and materials, all of which require innovative solutions complying with sustainability criteria.

In 2017 Portuguese exports increased circa 11 % reaching the highest value of the Gross Domestic Product (in a time horizon of 23 years). Portugal's Ministry of Economy estimates that capital-intensive industries (such as chemicals and polymers producers) and manufacturing industries (including food, textile, paper, cork, wood panels and metal producers) account for over 50 % of the overall value of the exportations. In this context, CHEMPOR 2018 emerges as a privileged forum to discuss technological and scientific issues that will promote economic growth through innovation.

The Organizing Committee accepted more than 345 communications, of which 83 oral presentations, after peer reviewing. Internationally recognized scientists were invited to deliver 6 Plenary Lectures and 6 Keynote Speeches. On the opening day of CHEMPOR 2018, the Portuguese Minister of Economy, Professor Manuel Caldeira Cabral, made a communication in the presence of dozens of industrial sponsors. Just before the closing session, the Professor Almiro Castro Award (sponsored by PARALAB) was granted , for the second time, and prizes were awarded to the best Oral and Poster Communications presented during the Conference.

The Organizing Committee of CHEMPOR 2018 acknowledges all authors for their contributions, all colleagues involved in the organization of the program, and the generosity of all sponsors.

We wish you a memorable Conference both scientifically and socially.

João A. P. Coutinho
(Chair of the Scientific Committee of CHEMPOR 2018)
(Full Professor of University of Aveiro)

Carlos Manuel Silva
(Chair of the Organizing Committee of CHEMPOR 2018)
(Associate Professor of Universidade de Aveiro)

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Program

Time		Tuesday, 2 /10			Wednesday, 3/10			Thursday, 4/10		
08:00	09:00	Registration								
09:00	09:15				**Plenary Lecture** *Rajamani Krishna* (PL3)			**Plenary Lecture** *Gabriele Centi* (PL5)		
09:15	09:30									
09:30	09:45	Welcome Session								
09:45	10:00									
10:00	10:15	**Plenary Lecture** *Nien-Hwa Linda Wang* (PL1)			O-BB07	O-EE01	O-IM03	O-RS11	O-EE10	O-BS05
10:15	10:30				O-BB08	O-EE02	O-IM04	O-RS12	O-EE11	O-BS06
10:30	10:45				O-BB09	O-EE03	O-IM05	O-RS13	O-EE12	O-BS07
10:45	11:00				O-BB10	O-EE04	O-IM06	O-RS14	O-EE13	O-BS08
11:00	11:15	Coffee-break			O-BB11	O-EE05	O-IM07		O-EE14	O-BS09
11:15	11:30				Coffee-break			Coffee-break		
11:30	11:45	O-RS01	O-BS01	Bondalti						
11:45	12:00	O-RS02	O-BS02	O-MP01	O-BB12	O-EE06	O-ME01	**Plenary Lecture** *Nikolaos Hadjichristidis* (PL6)		
12:00	12:15	O-RS03	O-BS03		O-BB13	O-EE07				
12:15	12:30	O-RS04	O-BS04	Prio	O-BB14	O-EE08	O-ME03			
12:30	12:45	O-RS05	O-BB01	O-IM01	O-BB15	O-EE09	O-ME04			
12:45		Lunch			Lunch			Lunch		
	14:15									
14:15	14:30	**Keynotes** *João Rocha* (KN1) *Rosa Quinta-Ferreira* (KN2)			**Keynotes** *Adélio Mendes* (KN3) *José António Teixeira* (KN4)			**Keynotes** *Maria Ascensão Reis* (KN5) *Ramesh Gardas* (KN6)		
14:30	14:45									
14:45	15:00									
15:00	15:15	O-RS06	O-BB02	BB&G	**Plenary Lecture** *María José Cocero* (PL4)			O-RS16	O-EE15	O-IM11
15:15	15:30	O-RS07	O-BB03	O-MP03				O-RS17	O-EE16	O-IM12
15:30	15:45	O-RS08	O-BB04	BP				O-RS18	O-EE17	O-IM13
15:45	16:00	O-RS09	O-BB05	O-MP04				O-MP05	O-IM09	O-IM14
16:00	16:15	O-IM02	O-BB06	O-RS10	Poster Session and Coffee-break P-BB, P-RS, P-MP, P-ME			O-IM08	O-IM10	O-IM15
16:15	16:30	**Plenary Lecture** *Paul Christakopoulos* (PL2)						Awards and Closing Session		
16:30	16:45									
16:45	17:00							Multibiorefinery Project Meeting Coffee-break (CHEMPOR participants are wellcome)		
17:00	17:15									
17:15	17:30	Formal Session with Minister of Economy								
17:30	17:45				Bus to Vista Alegre Museum Visit					
17:45	18:00									
18:00	18:15	Poster Session and Coffee-break P-BS, P-IM, P-EE								
18:15	18:30									
18:30	18:45									
18:45	19:00									
19:00	19:15									
19:15	19:30									
19:30					Conference Dinner					

[PL] - Plenary Lecture
[KN] - Keynote Presentation
[RS] - Reaction and Separation Processes
[BS]- Biorefinery and Sustainability
[MP] - Modeling, Synthesis and Integration of Chemical Processes

[BB] - Biological Engineering and Biotechnology
[IM] - Innovative Materials and Applications
[EE] - Energy and Environment
[ME] - Multiscale and Multidisciplinary Engineering Education

Index

Plenary Lectures [PL]

Keynotes Presentations [KN]

Oral session | Biological Engineering and Biotechnology [O-BB]

Oral session | Biorefinery and Sustainability [O-BS]

Oral session | Reaction and Separation Processes [O-RS]

Oral session | Energy and Environment [O-EE]

Oral session | Innovative Materials and Applications [O-IM]

Oral session | Modeling, Synthesis and Integration of Chemical Processes [O-MP]

Oral session | Multiscale and Multidisciplinary Engineering Education [O-ME]

Poster session | Biological Engineering and Biotechnology [P-BB]

Poster session | Biorefinery and Sustainability [P-BS]

Poster session | Reaction and Separation Processes [P-RS]

Poster session | Energy and Environment [P-EE]

Poster session | Innovative Materials and Applications [P-IM]

Poster session | Modeling, Synthesis and Integration of Chemical Processes [P-MP]

Poster session | Multiscale and Multidisciplinary Engineering Education [P-ME]

PLENARY LECTURE SPEAKERS

Professor Gabriele Centi

Gabriele Centi is full professor of Industrial Chemistry at the University of Messina, Italy, and President of the European Research Institute of Catalysis (ERIC). Research interests are in the areas of applied heterogeneous catalysis, sustainable energy and chemical processes, biomass conversion and environment protection.

He was coordinator of the EU Network of Excellence IDECAT, and is actually President of IACS (International Association of Catalysis Societies) and vice-President of the InterUniversity Consortium on the Science and Technology of Materials (INSTM). He was coordinator or PI in over twenty EU projects, besides many other national and industrial projects. He received several awards, and is involved in various editorial activities, between which chairing the editorial board of *ChemSusChem* and be co-editor in chief of *Journal of Energy Chemistry*. He was chairperson of many international conferences (the last one Europacat 2017 in Florence) and also chaired the 1st World Congress on Environmental Catalysis in Pisa (Italy) on May 1995. He is author of over 450 scientific publications, 12 books and editor of various special issues. Current h-index is 76 with about 21 250 citations (Google Scholar).

Professor Paul Christakopoulos

Paul Christakopoulos works in the area of Biochemical Process Engineering focusing on the development of biochemical (Green Chemistry) processes for the production and refinement of chemicals, fuels and material from CO_2, either captured before it is emitted to the atmosphere (non biomass route) or by recovering it from the atmosphere via photosynthesis in the form of biomass (biomass route). More specifically his research is focused on cellulose and lignin biorefinery, novel enzymes for modification of plant cell wall material, biocatalysis in non-conventional media, production of prebiotic oligosaccharides, production of biofuels and chemicals, biocatalytic CO_2 capture and conversion to chemicals and fuels. Paul has been appointed Chair Professor of Biochemical Process Engineering at Luleå University of Technology, Sweden, from February 2012. He has previously served as a Professor of Industrial Biotechnology at the School of Chemical Engineering, National Technical University of Athens.

He is author of over 230 scientific publications. Current h-index is 50 with about 7600 citations (Google Scholar). Paul had served as an Associate Editor of World Journal of Microbiology and Biotechnology, Food and Bioproducts Processing, PeerJ, Frontiers in Microbiology, FEMS Microbiology Letters.

Professor María José Cocero Alonso

María José Cocero Alonso is currently a Professor in the Department of Chemical Engineering and Environmental Technology at the University of Valladolid in Spain. She is director of the research group on High Pressure Process Engineering (http://hpp.uva.es/), and regional editor of The Journal of Supercritical Fluids. Her research is focused in processes and products contributing to the development of bio-economy, as (i) alternative use of natural resources for the production of chemicals and energy by subcritical/supercritical water, (ii) production of health related and high added value formulations from renewable raw materials by supercritical carbon dioxide, and (iii) intensification of processes through implementation of new technologies for upgrading raw materials and waste. She teaches master courses in supercritical fluids separation and reaction processes, and chemical engineering products.
María José Cocero Alonso published over 235 articles with ca. 5200 citations and h-index 38 (SCOPUS).

Professor Nien-Hwa Linda Wang

Professor N-H Linda Wang is the Maxine Spencer Nichols Professor of Chemical Engineering, Purdue University. She joined Purdue faculty in 1980 as the first female professor in Chemical Engineering. She received her BS in Chemical Engineering from National Taiwan University in 1971, her MS in Chemical Engineering from the University of Wyoming in 1973, and her PhD in Chemical Engineering from the University of Minnesota in 1978. She is a Fellow of the American Institute of Medical and Biological Engineering and a Fellow of the American Institute of Chemical Engineers (AIChE). She was a Director of the Separations Division, American Institute of Chemical Engineers (2001-2004) and a Director of the International Adsorption Society (2001-2007). She was the Chair of Separations Division of the AICHE in 2013. She is well respected as a leader in separations. She consulted for NSF, NIH, several national labs and many chemical, food, and pharmaceutical companies.

She is internationally known for her research contributions in adsorption, ion exchange, multicomponent chromatography, and simulated moving bed technologies. She has two patents, four patent applications, more than 120 technical publications, and more than 200 invited lectures and presentations at national and international meetings.

She is a leading expert in adsorptive separation methods. She made major contributions and published extensively in multicomponent chromatography and simulated moving bed (SMB) technologies for separating complex mixtures. She invented the seminal Standing Wave Design method for SMB processes. She developed the VERSE simulation software package, which is a powerful tool for understanding quantitatively adsorption and reaction phenomena in such processes. Recently she developed the first graphical solutions, which can be used to design affinity chromatography processes without any simulations.

In addition to her significant contributions to the fundamentals of chromatography, she developed the first tandem SMB process for insulin purification, and the first five-zone SMB for the recovery of six sugars from biomass hydrolysates. Recently she also developed a new capture chromatography process for the production of an important medical isotope. She developed the first separation process to recover polycarbonates and flame retardants from electronic wastes. She also developed the first ligand assisted chromatography method based on inorganic adsorbents for the production of high-purity rare earth elements. These new methods are expected to have a major impact on the environment and on the production of important chemicals and biochemicals.

Professor Nikos Hadjichristidis

Nikos Hadjichristidis is a Distinguished Professor of Chemical Sciences at King Abdullah University of Science and Technology, Saudi Arabia, and Emeritus Professor at the University of Athens, Greece.

The research of Professor Hadjichristidis focuses mainly on the synthesis of novel homopolymers and copolymers with well-defined complex macromolecular architectures, by using anionic polymerization (AP) high vacuum techniques as well as, combination of AP with other polymerizations (C1 and C3, ROP, ROMP, ATRP, etc.). These polymers are ideal models for checking the theory (e.g. de Gennes tube theory and hierarchical motion theory in branched polymers), understanding/improving the performance of industrial polymers (e.g. PE and PMMA), and are potential candidates for high-tech applications (e.g. nanolithography, high temperature membranes and drug delivery). Also his research interest includes the synthesis of hybrids of polymers with polypeptides, CNTs, silica and Au nanoparticles by using surface initiating polymerizations (anionic and C1) in order to overcome their inherent insolubility and make these materials more useful in nanotechnology applications. He has published more than 500 scientific papers in referred scientific journals (citations until May 31th 2018: 19990, h-index: 69, Web of Science; citations: 20160, h-index; 69, Scopus; citations: 27300, h-index: 78, Google Scholar), 25 patents, is the editor of three books and author of one book on “Block Copolymers” (Wiley 2003). Professor Hadjichristidis has received several awards including the *Macro Group United Kingdom Medal for Outstanding Achievements* (2016), the *ACS National Award for Polymer Chemistry* (2015), the *ACS Rubber Division Chemistry of Thermoplastic Elastomers Award* (2011), *the ACS Polymeric Materials Science and Engineering* (PMSE) *Division Cooperative Research Award* (2010), and the *International Award of the Society of Polymer Science*, Japan (SPSJ, 2007).

Professor Rajamani Krishna

Rajamani Krishna received his PhD degree in Chemical Engineering in 1975 from the University of Manchester in England, and soon thereafter joined the Royal Dutch Shell Laboratories, Amsterdam in The Netherlands. At Shell, he was involved in a wide range of research and developmental activities in separations and reaction processes. Since 1990, he is Professor at the Van ‘Hoff Institute for Molecular Sciences, University of Amsterdam.

Professor Krishna's research interests range from molecular modelling, bubble and particle dynamics to reactor scale up to process synthesis. The main goal of this research concerns the development of unifying concepts in multicomponent diffusion and multiphase hydrodynamics, both in separations and reaction engineering. He has pioneered the development of the Maxwell-Stefan diffusion formulation and its application to fluid phases, porous solids, and complex three-phase (vapour-liquid-liquid) systems. The Krishna Group has investigated the hydrodynamics of various types of multiphase reactors, using the Computational Fluid Dynamics technique. Improved design procedures have been developed for bubble columns, slurry and air-lift reactors, gas-solid fluidized beds, catalytically structured reactors, distillation trays, and catalyst containing trays. Professor Krishna has also contributed to the understanding of the influence of low-frequency sound waves on gas and liquid flow in bubble columns.

The current focus of Krishna's research is on development of novel energy-efficient separation technologies using ordered crystalline nanoporous adsorbents.

Thanks to his wide experience, based both on his academic and industrial careers, Professor Krishna is recognised worldwide as a leading scientific expert. He has received several awards, which include the prestigious CONRAD Prize of the Dutch Institute of Engineers, and the Akzo Nobel Science Award. He is the recipient of the prestigious 2013 ENI award in the category New Frontiers of Hydrocarbons (Downstream) for his research theme Improving Process Technologies with Molecular Insights.

Krishna is included in the 2017 list of the most Highly Cited Researchers (category: Chemistry); see https://clarivate.com/hcr/2017-researchers-list/.

He has published more than 500 peer-reviewed journal articles, and two text books, one of which has been translated into Chinese. He holds several patents. A complete list of his research contributions can be found on Google Scholar; see http://scholar.google.nl/citations?user=cKqtQ0MAAAAJ&hl=en. His publications have been cited more than 36 000 times, with an h-index of 101 (Google scholar).

KEYNOTE SPEAKERS

Adélio Mendes

Professor Adélio Mendes (born 1964) received his PhD degree from the University of Porto in 1993, and is currently Full Professor at the Department of Chemical Engineering of the Faculty of Engineering - University of Porto. Coordinates a large research team with research interests mainly in dye sensitized solar cells and perovskite solar cells, photoelectrochemical cells including water splitting and solar redox flow batteries, photocatalysis, redox flow batteries, electrochemical membrane reactors (PEMFC, H-SOFC, chemical synthesis), methanol steam reforming, membrane and adsorbent-based gas separations and carbon molecular sieve membranes synthesis and characterization.

Professor Mendes authored/co-authored ca. 330 articles in peer-review international journals, possesses nearly 5970 citations and h-index 38. He filled 23 families of patents and is the author of a textbook. He received an Advanced Research Grant from the ERC on dye-sensitized solar cells for building integrated of ca. 2 M€ and since 2013 he is partner in 2 more EU projects leading one of them. He received the Air Products Faculty Excellence 2011 Award (USA) for developments in gas separation, Solvay & Hovione Innovation Challenge 2011 prize, the Prize of Coimbra University of 2016, and the prize of Technology Innovation - 2017 by the University of Porto. Presently, he is the Coordinator of CEner-FEUP, the Competence Center for Energy of the Faculty of Engineering at the University of Porto.

João Rocha

João Rocha is Full Professor of Inorganic and Materials Chemistry at the Department of Chemistry, University of Aveiro, and Director of CICECO - Aveiro Institute of Materials. He is member of the European Academy of Sciences (EURASC) and of the Lisbon Academy of Sciences, and Fellow of Royal Society of Chemistry and of the ChemPubSoc Europe. He has received the Madinabeitia-Lourenço award from the Real Sociedad Española de Química, the prize Ferreira da Silva (Portuguese Chemical Society), and the prize for Scientific Excellence from the Portuguese Science Foundation. He was member of the National Science and Technology Council (advising the Prime Minister). He headed the Commission on Inorganic and Mineral Structures of the International Union of Crystallography and is consultant for the Commission on NMR Crystallography and Related Methods. Professor João Rocha published ca. 490 SCI papers and 24 book chapters with ca. 16,000 citations (h-index 60) and 4 patents; gave over 200 talks at conferences; and supervised 40 post-docs and 25 PhDs. His present main research interests encompass microporous transition metal and lanthanide silicates, photoluminescent lanthanide-bearing materials, and Metal Organic Frameworks for sensing applications, including nanothermometry; nanosystems for multimodal (magnetic resonance, optical and thermometry) imaging and small molecules drug delivery; solid-state NMR and X-ray diffraction.

José António Teixeira

José António Teixeira is currently full Professor at Biological Engineering Department, University of Minho (since 2000). He has a degree in Chemical Engineering from University of Porto (1980) and a PhD in Chemical Engineering also from University of Porto (1988). He has been involved in different management activities, being Head of the Department of Biological Engineering, Univ. Minho, 2000-2012, and Head of Biological Engineering Research Centre, 2012-2015.

Prof. José Teixeira has a wide research expertise in Industrial Biotechnology (bioprocess development for the transformation of lignocellulosic materials into 2nd generation bioethanol and chemicals; valorization of agro-industrial residues; bioreactor development and continuous processing) and Food Biotechnology (non-conventional food processing; edible films for packaging; food nanotechnology, process development for production of prebiotics).

He was responsible/co-responsible for the supervision of 31 PhD theses and 20 Post-docs and has been the coordinator of 32 scientific research projects, 7 of which international. José Teixeira was awarded the “Stimulus to Excellence”, 2006, from FCT, the “Seeds of Science” in “Engineering and Technology”, 2011, from “Ciência Hoje” and the “Scientific Merit Award”, Universidade do Minho, 2015. He is the co-editor of the books “Reactores Biológicos-Fundamentos e Aplicações” (in Portuguese), Engineering Aspects of Milk and Dairy Products and Engineering Aspects of Food Biotechnology, and the author/co-author of over 535 peer reviewed papers with more than 14260 citations and h-index 58.

Maria da Ascensão Reis

Maria Reis is a Full Professor in Environmental Biotechnology at FCT-NOVA. Main research interests have been in the area of Environmental/Industrial Bioengineering, with special focus on the development of sustainable bioprocesses for the removal of pollutants from water and wastewater streams and for the exploitation of industrial wastes for the production of biopolymers and bulk chemicals. Within this research area, published more than 220 papers in scientific journals with peer review, possesses around 7070 citations and h-index 44. She is the co-author of 18 Book Chapters. Presented more than 200 oral presentations in International conferences. Is co-author of 4 National patents and 6 International patents. Coordinated 20 national and international projects (team leader), out of which 12 European Projects and 6 were co-funded by industrial companies, and participated as team member in 22 research projects. Co-supervised 20 PhD students and is currently co-supervisor of 11 PhD students. Her scientific work has been distinguished with several awards and she was the winner of the Solvay & Hovione Ideas Challenge SHIC’08 Prize- Solvay prize in 2008. Nominated and Elected to the Portuguese Academy of Engineering in 2009 and Elected as IWA Fellow, September 2010. She is Editor of the Water Research (Elsevier).

Ramesh L. Gardas

Ramesh Gardas was born and brought up in Surat, Gujarat, India. He completed B.Sc. (Chemistry) with First Class from P.T. Sarvajanik College of Science, Surat in 1998 and M.Sc. (Physical Chemistry) with First Class from Department of Chemistry, South Gujarat University, Surat in 2000. He has been awarded the Ph.D. degree in Chemistry in 2004 by the Veer Narmad South Gujarat University, India, for his work on thermodynamic studies of non-electrolyte binary and ternary liquid mixtures under the supervision of Prof. S.L. Oswal. Then, he joined the research group of Prof. Abel Ferreira and Prof. Isabel Fonseca at the University of Coimbra, Portugal, for his first post-doc research on PVT data of pure and binary liquid mixtures. Later, in 2006, he joined University of Aveiro, Portugal, to work with Prof. João Coutinho and Prof. Isabel Marrucho. His second post-doc focused on water solubility, octanol-water partition coefficients, and thermophysical properties prediction of ionic liquids. Then, in May 2008, he moved to Queen's University Belfast, Belfast, UK, and joined the QUILL Research Team to work with Prof. Chris Hardacre and Prof. David Rooney for his third post-doc on confidential project sponsored by Petronas, Malaysia. Research experience from Aveiro and QUILL improved his knowledge of ionic liquids and more precisely their physico-chemical properties and applications. He joined the Indian Institute of Technology Madras, India, in August 2010, as an Assistant Professor in Chemistry and promoted to Associate Professor in July 2015. He has more than 18-years of research and 8-years teaching experience. He is a co-author of 4 patents, 2 book chapters and 143 research papers with ca. 3900 citations with h-index 30 (SCOPUS).

Rosa Quinta-Ferreira

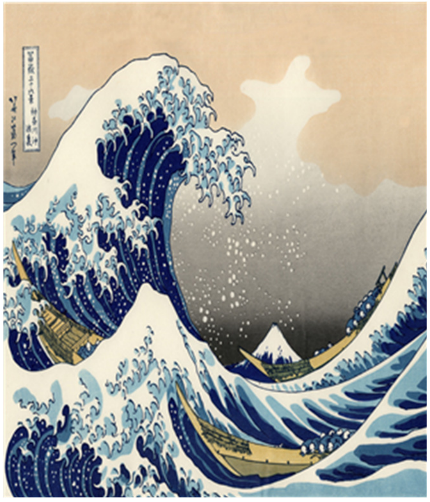
Rosa Maria de Oliveira Quinta Ferreira, name for scientific publications Rosa M. Quinta-Ferreira, was born in 1952, graduated in Chemical Engineering at the University of Coimbra, Portugal, in 1975, received the DEA - Diplome d'Études Approffondies - from the Université Pierre et Marie Curie, Paris, France, in 1981 and the PhD degree in Chemical Engineering from the University of Porto, Portugal, in 1988 and had the Aggregation degree in 2015. Full Professor in the Department of Chemical Engineering at the University of Coimbra since 2018 and Coordinator of the Group on Environment, Reaction, Separation and Thermodynamics (GERST) of the Chemical Processes Engineering and Forest Products Research Centre (CIEPQPF) of the University of Coimbra. Published 143 papers in specialized scientific journals with ca. 1800 citations, 15 chapters of books and 210 communications to scientific meetings. Supervised 11 PhD thesis, 34 Master thsesis and co-supervised 3 besides the supervison of 91 final scientific dissertations for graduation in chemical engineering in the pre-Bologna period (equivalent to the actual master thesis). Principal investigator of 9 financed projects by the Research National Foundation (FCT) and researcher in 6 other national projects. As coordinator of the UC team, integrated a transnational bilateral cooperation project, was member of the team of an EU FP6 project and an EU FP7 project and is member of a POCTEP Portugal-Spain project. The general research specialization domain is Reaction Engineering, including computational modeling, through phenomenological models and advanced Computational Fluid Dynamics (CFD) frameworks, as well as experimental work dedicated to the environmental preservation from polluted liquid, gas and solid wastes. In particular, Advanced Oxidation Processes (AOPs) for liquid effluents treatment have been developed under the common denominator of heterogeneous catalysis, including wet oxidation, ozonation, Fenton's, photo-assisted systems and electrochemical processes. Spin-off companies were created from her research group with the support of the research carried out in her laboratorial facilities. Advanced Biotechnology Processes embrace novel solutions for environment safeguarding. For VOCs decontamination, autothermal systems are investigated, whereas fly ashes recycling and composting methodologies are targeted as solid wastes valorization. Chemical, Environment and Biotechnology Reaction Engineering are joint domains to search sound environmental technologies for the planet remediation. Health concerns about the effect of biological and chemical contaminants on public welfare are reinforced within multidisciplinary pharmaceutical, biophysics and medical sciences areas.

PLENARY LECTURES

[PL01]

Simulated moving beds: Fundamental principles, enabling technologies, and applications

N.-H.L. Wang
Davidson School of Chemical Engineering, Purdue University. 480 Stadium Mall Drive, West Lafayette, Indiana, USA.
** wangn@ecn.purdue.edu*

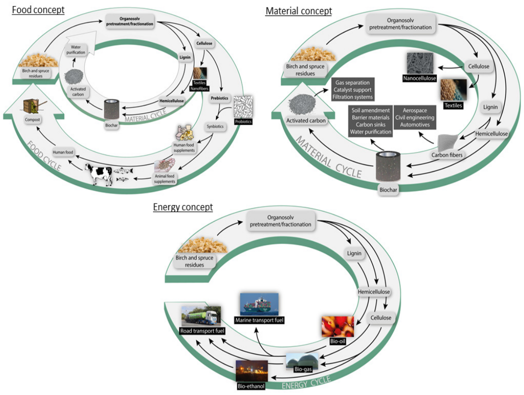


Chromatography methods are highly selective separation methods, which are used for manufacturing many chemicals and biochemicals. Simulated moving beds (SMBs) are advanced continuous chromatography methods, which are more efficient and can have one or two orders of magnitude lower manufacturing costs than conventional batch chromatography. SMB methods, however, are not widely taught in conventional science or engineering curricula. SMB processes designed empirically usually have low yield, productivity, and solvent efficiency. In this talk, the fundamental principles of SMB and two key tools, a rate model simulation tool (VERSE) and the Standing Wave Design and Optimization tool (SWD), will be briefly introduced. The tools can be used to help understand, analyze, simulate, design, optimize, and develop various types of SMBs. Three examples will be used to show the applications of the tools: (1) a tandem SMB for the purification of insulin from a ternary mixture, (2) a five-zone SMB for the recovery of six sugars from biomass hydrolysates, and (3) a three-zone non-isocratic SMB for protein capture or purification.

[PL02]

Novel hybrid organosolv: Steam explosion-based integrated biorefinery of the lignocellulosic biomass (an evolution from pretreatment to fractionation processes)

P. Christakopoulos*, L. Matsakas, A. Karnaouri, A. Patel, U. Rova
Biochemical Process Engineering, Department of Civil, Environmental and Natural Resources Engineering, Luleå University of Technology, SE-97187, Luleå, Sweden.
** paul.christakopoulosr@ltu.se*



A novel biomass pretreatment was established in the current work, which combines the fractionation efficiency of the traditional organosolv cooking with the size reduction and improvement of the hydrolysability that steam explosion offers. This hybrid method was applied on both hardwood (birch) and softwood (spruce) biomass where various process parameters were optimized toward achieving high fractionation efficiency. The pretreated solids presented superior hydrolysability, allowing their use to various biotechnological applications such as ethanol fermentation, biogas, microbial oil and cellulooligosaccharides production. High purity lignin was also isolated permitting its use in advanced applications such as nanoparticles formation and as lubricant additive. The newly established hybrid method can play a significant role towards the establishment of a biomass biorefinery, allowing the use of all biomass components for the production of fuels, chemicals and materials.

[PL03]

Exploiting entropy effects in separations with microporous crystalline adsorbent materials

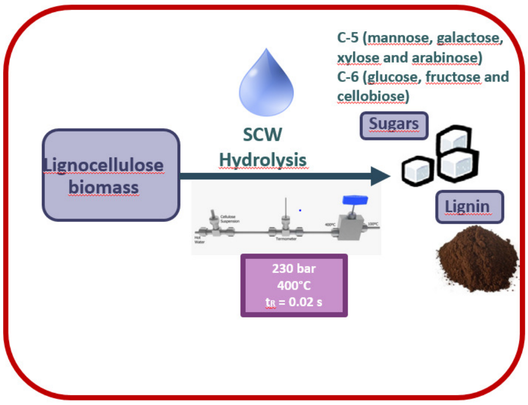
R. Krishna
Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, 1018 WV Amsterdam, The Netherland.
r.krishna@contact.uva.nl

The most commonly used adsorption separation strategies involve distinguishing molecules on the basis of (a) size and mobility, (b) van der Waals interactions and polarizability, (c) electrostatic interactions, and (d) π-electron transfers. The use of ordered crystalline microporous materials, such as zeolites (crystalline aluminosilicates), metal-organic frameworks (MOFs), and zeolitic imidazolate frameworks (ZIFs), with channel dimensions in the 3 Å – 20 Å range, opens up new separation strategies that are not realizable with amorphous adsorbents. Particularly noteworthy are possibilities of separations on the basis of subtle differences in molecular configurations, and efficiencies with which molecules pack or stack within the microporous channels. Packing effects are of particular importance in separations of mixtures that operate under conditions of pore saturation. Broadly speaking, the component that is preferentially adsorbed is the one that packs most efficiently; this preference may be rationalized by $S = k_B \ln(W)$. My talk will highlight a wide variety of industrially important separations that exploit entropy effects. The examples considered include separations of mixtures of (a) hexane isomers, (b) xylene isomers, (c) linear alkanes, and (d) linear alcohols.

[PL04]

Overcoming the challenges of the sustainable biorefinery: Supercritical water ultrafast processes

M.J. Cocero
Valladolid University. BioEcoUVa Research Institute (Spain).
mjcocero@iq.uva.es



The concept of biorefinery was proposed already in the late 1980s but the cost and complexity of processing biomass have impaired is implementation so far. The fractionation of biomass into its components poses a major challenge, because the recalcitrance of the lignocellulose matrix makes typical feedstock difficult to fractionate. Another challenge is the production of aromatics; much fundamental research has focused on lignin transformation to aromatics, but little of this effort has been transformed into products close to market.

SCW is a solvent and reaction medium that could solve these challenges. The SCW ultrafast process allows to:

- improve the selectivity of the hydrothermal processes by understanding the SCW biomass fractionation fundamentals;
- produce liquid effluent with a high concentration of sugars and a solid effluent that is mainly lignin;
- transform 60% of the lignin in oil, with 20% of key aromatics and 4% of char.

[PL05]

Beyond fossil fuels for a transformative energy and chemistry

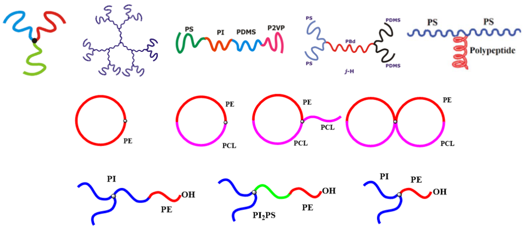
G. Centi*, S. Perathoner
Dept.s ChiBioFarAm and MIFT – Chimica Industriale, University of Messina (Italy), INSTM/CASPE and ERIC aisbl, V.le F. Stagno D'Alcontres 31, 98166 Messina, Italy.
** centi@unime.it*

In the last few years, a new theme is becoming of increasing relevance, driven in part from sustainable (mitigate climate change) and geopolitical (security and diversification of resources) motivations, but now largely from economic ones: make chemistry and energy without fossil fuels. It is thus necessary to reconsider the possibilities to make base chemicals from alternative sources, waste materials being clearly on obvious choice also in consideration of a circular economy, and to look also at the role of chemical energy storage in this renewable energy panorama.[1,2] The lecture will first analyze the scenario opened from this transition to a new (sustainable and low carbon) chemistry and energy, in relation to the change in their nexus and related influence on economics. It will then discuss some options for a short, medium and longer term change. For short term, the use of waste as alternative C-source is discussed,[3] with an analysis of the waste to chemical possibilities and an analysis of the role of chemical energy storage to enable the transition to a renewable-energy-driven economy.[4] For medium- and longer-term, the role of electrocatalytic and photo-electro-catalytic technologies, the latter in relation to the development of artificial-leaf type devices, is discussed.

[PL06]

The importance of model polymers in polymer science and industry

N. Hadjichristidis
King Abdullah University of Science and Technology, Physical Science and Engineering Division, Catalysis Center, Polymer Synthesis Lab., Saudi Arabia.



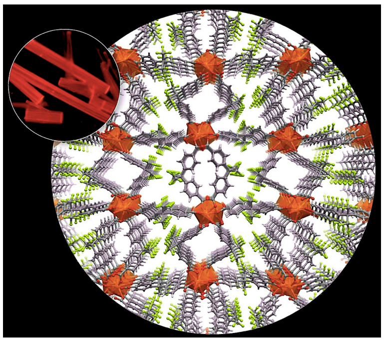
Access to model polymers (high degree of structural, compositional and molecular weight homogeneity) is necessary in order to elucidate structure-property relationships, which are the key in improving polymer performance and designing new materials. The synthesis of model polymers with different structures (a few are given in Figure 1) is demanding, time consuming and often leads to a small quantity of products [1-3]. Nevertheless, this is a small price to pay given the tremendous potential of model macromolecules for selecting the appropriate structures needed for specific applications. Among others these model polymers serve in: Better testing existing theoretical concepts; Developing new theoretical concepts to explain experimental results on novel structures; Understanding/Improving the properties of industrial polymers.

KEYNOTE PRESENTATIONS

[KN01]

The importance of being porous: Silicates and functional Metal Organic Frameworks

J. Rocha
University of Aveiro, CICECO - Aveiro Institute of Materials, Department of Chemistry, Aveiro, Portugal.
rocha@ua.pt

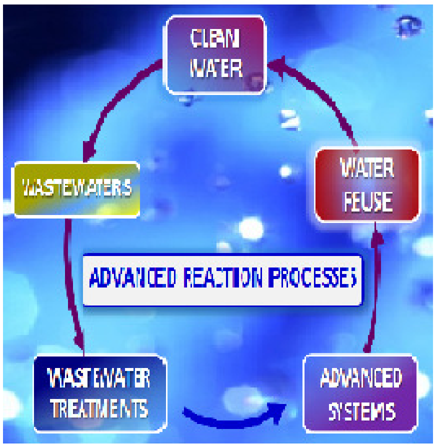


Some of the work carried out in Aveiro on nanoporous transition-metal and lanthanide (Ln) silicates, and on Ln-bearing coordination polymers (or metal organic frameworks, MOFs) will be reviewed.

[KN02]

Advanced reaction processes, wastewater treatment and reuse

R.M. Quinta-Ferreira
CIEPQPF – Chemical Engineering Processes and Forest Products Research Center, Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, Pólo II – RuaSílvio Lima, 3030-790 Coimbra, Portugal.
rosaqf@eq.uc.pt



Water supplies from natural resources are reaching dramatic low levels imposing high stress on the water quality available for human activities. Polluted streams returning to the environment after usage in domestic and industrial systems are leading to contaminants accumulation in lakes and rivers. Lack of fresh water is therefore pushing scientists, governments and society to become aware of the need to properly treat wastewaters targeting their reuse. Novel treatments urge then to be found to fulfill environment legislations aiming at water recycling. Chemical Reaction Engineering has a fundamental role in this domain through the proposal of advanced reaction processes able to produce strong oxidant species such as the hydroxyl radicals. Heterogeneous catalysis is also crucial for improving the efficacy of such technologies ensuring adequate catalysts separation. The high diversity of effluents claims a large spectrum of reactor types aiming to tailor the best solutions to specific treatments.

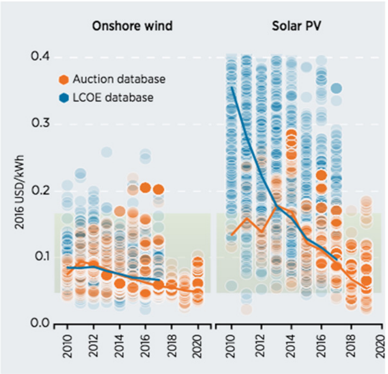
[KN03]

Harvesting and storage of solar energy: a promising new world for off the grid residences?

A. Mendes

LEPABE - Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.

mendes@fe.up.pt



Source: IRENA Renewable Cost Database and Auctions Database.

The photovoltaic (PV) electricity is expected to reach the lowest price of fossil fuel electricity by 2020 and below that reference price after 2020. Obviously that the actual price of the PV electricity depends on the production location and in Portugal the PV electricity is already cheaper than the fossil fuel electricity.This remarkable achievement is fueling the development and use of technologies for harvesting energy from renewable sources using namely photovoltaic panels and wind mills. Compared to the fossil fuel electricity, PV electricity is not dispatchable making necessary the combined use of storage systems. A worldwide tremendous effort is now being developed for producing stationary battery systems suitable for handling electricity from renewable sources, which display intermittence. Redox flow batteries are taking the lead for storing energy easily and efficiently transformed in electricity.

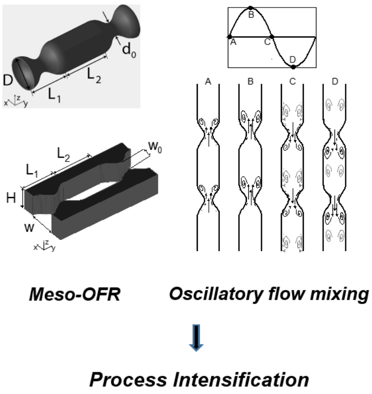
[KN04]

Oscillatory Flow Reactors – A platform for process intensification

J.A. Teixeira

CEB - Centre of Biological Engineering, University of Minho, 4710-057 Braga, Portugal

jateixeira@deb,uminho.pt

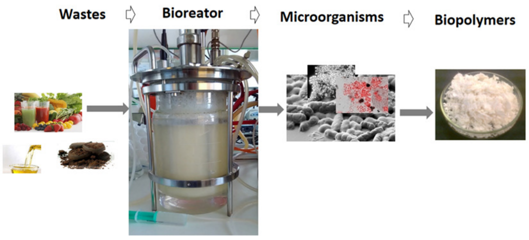


Process intensification demands the development of innovative and more sustainable process design alternatives in order to tackle the challenges related with mixing efficiency. OFR – oscillatory flow reactor – have been proposed as an alternative design to overcome these limitations. OFR, basically a column provided with periodic sharp constrictions, operated under oscillatory flow, have shown to improve significantly processes where mixing is relevant. The application of OFR to several processes will be presented and perspectives for its development discussed

[KN05]

Shifting organic waste paradigm: From accumulation to valorisation into biopolymers

M. Reis
UCIBIO, REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal.
amr@fct.unl.pt



The wide use of biodegradable biopolymers has been limited by the cost. The use of wastes or industrial by-products as substrate is the most promising strategy to reduce the cost of microbial biopolymers and make them more competitive. An overview of strategies for the production of biopolymers from wastes at lab to pilot scale will be presented, with the main focus on the production of polyhydroxyalkanoates (PHA) and polysaccharides using pure and mixed cultures.

[KN06]

Utilizing ionic liquids as additives for enhancing the extraction, absorption and dissolution processes

R.L. Gardas
Department of Chemistry, Indian Institute of Technology Madras, Chennai 600 036, India.
gardas@iitm.ac.in

Solvents are major contributors and high on the list of environmental damage chemicals, mainly because of their large usage and high volatility. The widespread use of volatile organic compounds (VOCs) in many industrial chemical processes is an issue of great environmental concern. It is an extremely important task to search of potentially green and environment friendly alternatives for VOCs. At least a partial solution to this problem may offer by a novel class of molten salts referred to as ionic liquids (having melting point, generally, below boiling point of water), as they possess unique combination of particular properties, unlike molecular liquids, namely negligible vapour pressure (~ 10^{-11} to 10^{-10} bar at room temperature), wide thermal window (~ -50 °C to +250 °C), wide electrochemical window (~ ±3 Volt vs. NHE), non-flammability, high ionic conductivity and a highly solvating capacity for organic, inorganic and organometallic compounds. This unique combination of particular properties leads them to be exploited as “green solvents” and giving them increasing attention in academic and industrial research.

paralab

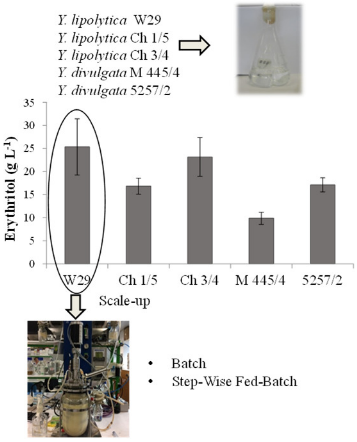
Oral Session

BIOLOGICAL ENGINEERING AND BIOTECHNOLOGY

[O-BB01]

Production of erythritol by *Yarrowia* species from crude glycerol

P. Ferreira[1*], *M. Ribeiro*[1], *A.R. Machado*[1], *E. Nagy*[2], *D.Q. Nguyen*[2], *I. Belo*[1]
[1] *CEB - Centre of Biological Engineering, University of Minho, 4710-057 Braga, Portugal.* [2] *Research Centre for Bioengineering and Process Engineering, Szent István University, Ménesi út 45, H-1118 Budapest Hungary.*
* *patricia.ferreira@ceb.uminho.pt*

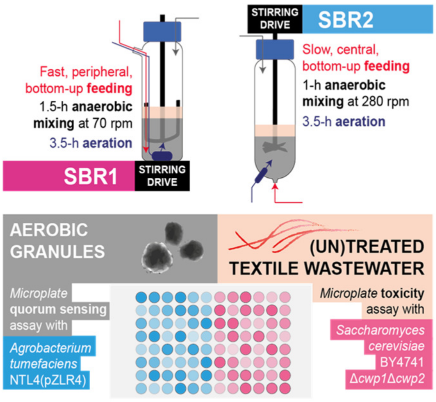


Erythritol is a four-carbon sugar alcohol that has about 70 % of the sweetness of sucrose. Erythritol is mostly produced by fermentation from glucose or glycerol using osmophilic fungi. In this work different strains and species of *Yarrowia* genus were evaluated for their ability to produce erythritol from crude glycerol, a byproduct of biodiesel industry. The performance of strains from *Y. lipolytica* and *Y. divulgata* species was compared in flasks batch culture. All strains were able to produce erythritol in the tested conditions. *Y. lipolytica* W29 strain presented the highest concentration, yield and productivity of erythritol. A scale-up to a lab-scale stirred tank bioreactor using two different operation modes, batch and step-wise fed-batch was performed. With the scale-up 3-fold increase on productivity was observed. In the step-wise fed-batch the addition of glycerol allowed to reach almost the double of erythritol concentrations (64 g L^{-1}).

[O-BB02]

Comparing the operation of aerobic granular sludge bioreactors under different hydrodynamic regimens during the treatment of textile wastewater containing silver nanoparticles

M.S. Coelho[1], *S. Sousa*[1], *A.M. Rodrigues*[1], *R.D.G. Franca*[1], *C.A. Viegas*[1], *H.M. Pinheiro*[1], *N.D. Lourenço*[1,2,*]
[1] *iBB – Institute for Bioengineering and Biosciences, Department of Bioengineering, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal;* [2] *UCIBIO, REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Campus de Caparica, 2829-516 Caparica, Portugal.*
**nidia.lourenco@fct.unl.pt*

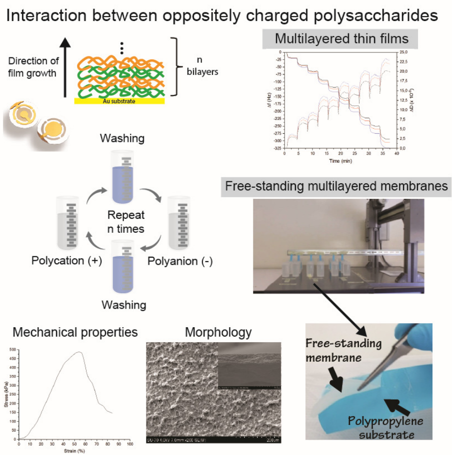


Two aerobic granular sludge (AGS) sequencing batch reactors (SBRs) were used in the treatment of a textile wastewater (TWW) containing an azo dye and silver nanoparticles and monitored for granule development and maintenance, *N*-acyl-homoserine lactone (AHL) content as a quorum sensing (QS) indicator and effluent detoxification. Each SBR was run using a different feeding strategy and hydrodynamic shear pattern to assess the impact of these operational conditions. The use of lower hydrodynamic shear was shown to benefit granule formation during the initial stages of the operation but became less relevant in time. AHL QS appeared to be an important feature of granulation, as well as the applied shear. However, biomass washout episodes in later stages led to the removal of AHL-producing bacteria and markedly reduced AHL. Overall, the two SBRs displayed similar performances in terms of TWW toxicity changes during treatment, model yeast growth being inhibited by over 60% after dye reduction.

[O-BB03]

Assessing the influence of the adsorption time on the build-up of natural-origin polymeric multilayered systems: how fast can we go?

T. Pesqueira[*], *J. Borges, J.F. Mano*
Department of Chemistry, CICECO – Aveiro Institute of Materials. University of Aveiro. Campus Universitário de Santiago. 3810-193 Aveiro, Portugal.
** tamagno@ua.pt*

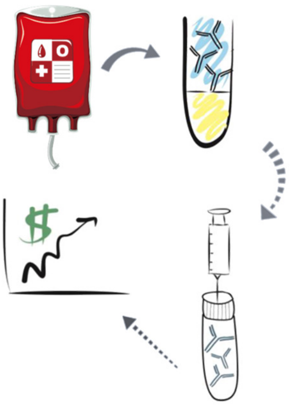


The Layer-by-Layer (LbL) approach is a straightforward technology to fabricate highly ordered multilayered architectures with applications in the biomedical field. However, physicochemical, biological and mechanical properties of the multilayered systems are greatly influenced by both intrinsic and extrinsic parameters, being pivotal to understand their influence at molecular level. This work investigates the effect of chitosan (CHT) and alginate (ALG) biopolymer adsorption and rinsing times on the physicochemical, biological and mechanical properties of CHT/ALG free-standing membranes. Different combinations of biopolymer deposition and rinsing times were studied regarding film thickness, mass deposited, swelling ability, mechanical and biological properties. This work demonstrates that membranes with similar properties can be quickly developed by extensively shortening the adsorption time needed for building blocks interaction, turning LbL technology more prone for commercial use.

[O-BB04]

Recovery of value-added antibodies from serum samples

E.V. Capela[1,2], *J.A.P. Coutinho*[1], *M.R. Aires-Barros*[2], *A.M. Azevedo*[2], *M.G. Freire*[1,*]
[1] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;* [2] *iBB - Institute for Bioengineering and Biosciences, Department of Bioengineering, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal;*
**maragfreire@ua.pt.*

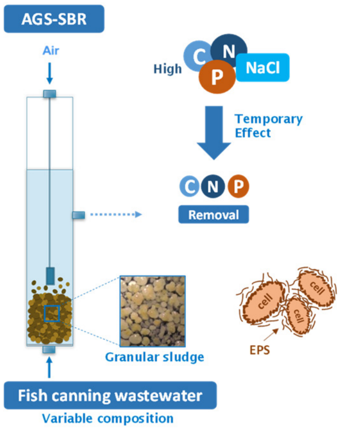


In this work, ionic-liquid-based aqueous biphasic (liquid-liquid) systems were applied in the downstream processing of antibody-based biopharmaceuticals, namely immunoglobulin G antibodies, from human serum samples. The nature of the phase-forming components and phases' compositions were investigated in order to selectively extract antibodies to the top phase, allowing to recover antibodies with a high purity level and integrity.

[O-BB05]

Aerobic granular sludge process treats real fish canning wastewater

A.M.S. Paulo[1,*], *C.L. Amorim*[1,2], *P.M.L. Castro*[1]
[1]*Universidade Católica Portuguesa, CBQF - Centro de Biotecnologia e Química Fina – Laboratório Associado, Escola Superior de Biotecnologia, Rua Arquiteto Lobão Vital, 172, 4200-374 Porto, Portugal;* [2]*Biology Department and CESAM, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal.*
* *apaulo@porto.ucp.pt*



Aerobic Granular Sludge (AGS) is an innovative technology used for carbon and nutrients removal from wastewater, using less space and energy compared to other biotechnological solutions. Aerobic granules present a compact structure, composed of extracellular polymeric substances (EPS), which increase AGS resistance to variable wastewater composition, as those commonly produced by industry. In this study, C, N and P-removal from a fish canning plant wastewater was evaluated using an AGS-SBR (sequential batch reactor). Throughout the first 3 months of operation with variable feed composition, the chemical oxygen demand (COD) at the outlet was below the discharge limit of 125 mg O_2 L^{-1}, phosphorous removal was stable and the nitrification process improved. At the higher organic loading rates (OLR), the AGS performance was temporary affected. This study contributes to understanding the effects of the variability of a real wastewater on an AGS process.

[O-BB06]

Water2Return: towards the total recovery of nutrients from the sewage water in a slaughterhouse

C. Aragon[1,*], *A. Real*[1], *I. Martin*[1], *K. Fahd*[1], *J. Parrado*[2], *P. Caballero*[2]
[1] *Fundacion CENTA. Autovia Sevilla-Huelva (A49) km 28. 41820. Carrion de los Céspedes, Spain;* [2] *Department of Biochemical and Molecular Biology, Faculty of Pharmacy, University of Seville, Spain.*
* *caragon@centa.es*

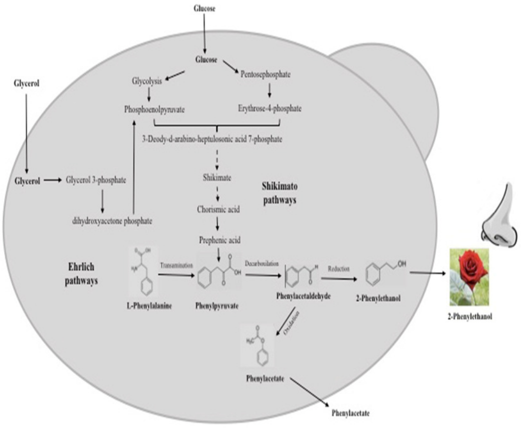
Nowadays, water scarcity and resource recovery are global concerns. Therefore, there is rising demand for alternative and sustainable solutions to use water in the best possible way and to recover resources from going to waste. These solutions become a must when dealing with industrial sectors like slaughtering, a water-intensive industry that generates wastewater containing a high proportion of organic matter. This wastewater can be a valuable source of nutrients if properly recovered.

Water2REturn project adopts a Circular Economy approach where nutrients present in wastewaters from the meat industry can be recycled and injected back into the agricultural system as new raw materials. Water2REturn proposes a full-scale demonstration process for integrated nutrients recovery using biochemical and physical technologies. The project also proposes innovative business models for the resulting products that will open new market opportunities in the environmental and agricultural sectors.

[O-BB07]

Yarrowia lipolytica as a potential producer of 2-phenylethanol from L-phenylalanine biotransformation

A. Braga[1,*], *A. Oliveira*[1], *B. Freitas*[1], *E. Nagy*[2], *D. Q. Nguyen*[2], *I. Belo*[1]
[1] CEB - Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710–057 Braga, Portugal [2]Research Centre for Bioengineering and Process Engineering, Szent István University, Ménesi út 45, H-1118 Budapest Hungary.
** abraga@deb.uminho.pt*

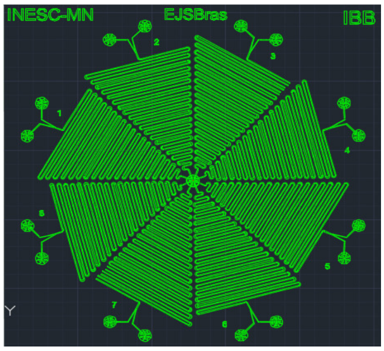


2-Phenylethanol (2-PE) is an aromatic alcohol with a delicate fragrance of rose petals. The non-conventional yeast *Yarrowia lipolytica* is extensively explored for flavor compounds production, but the production of 2-PE has been very poorly described. This study investigated the potential of different *Y. lipolytica* strains (W29, CBS2075, CH 1/5 and CH 3/4) for 2-PE production. It was confirmed that all strains were able to produce 2-PE by L-phenylalanine (L-Phe) bioconversion, but were inhibited by 2-PE concentrations above 2 g L^{-1}. The strain *Y. lipolytica* CH 1/5 was selected for further studies since it produced the highest 2-PE titer (2.2 g L^{-1}). Afterwards, the effect of L-Phe concentration and carbon source (glucose and crude glycerol) on 2-PE production was studied, and it was observed that increasing L-Phe concentration decreases the aroma production, and that the highest titer was obtained with glycerol. This study demonstrates the promising production of 2-PE using *Y. lipolytica* as biotechnological platform for flavors production.

[O-BB08]

A microfluidic platform for optimization of downstream process of biopharmaceuticals

*R. Aires-Barros**, *A, Azevedo*
IBB – Institute for Bioengineering and Biosciences, Instituto Superior Técnico, Department of Bioengineering, Universidade de Lisboa, Lisbon, Portugal.
** rabarros@ist.utl.pt*

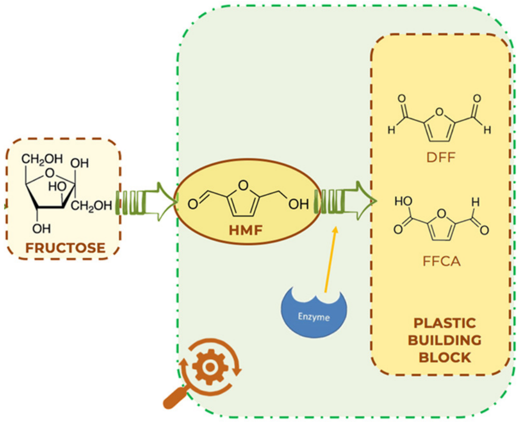


Miniaturization platforms as high-throughput screening tools to speed up process optimization are described.

[O-BB09]

Sustainable production of plastic building blocks by enzymatic biocatalysis

Y. Moldes-Diz*, F. Manteiga, G. Feijoo, M.T. Moreira
Universidade de Santiago de Compostela, ETSE, Rua Lope Gomez de Marzoa s/n, Santiago de Compostela, Spain.
* *yolanda.moldes@usc.es*

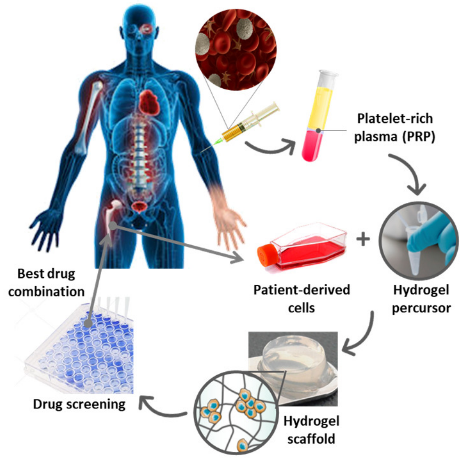


Galactose oxidase (GAO) and aryl alcohol oxidase (AAO) have been shown to be promising biocatalysts for the oxidation of primary and secondary alcohols. However, the use of free enzymes on an industrial scale presents low stability and the possibility of reusing the biocatalyst depends on the viability of separation of the free enzyme in ultrafiltration membrane systems. Different enzyme immobilisation strategies have been proposed, with the aim of improving activity and protein stability. This study presents different immobilization techniques for GAO and AAO on supports based on ionic interactions and covalent bonds: Agarose-glyoxyl, Relizyme, Lifetech ECR8204/F, Lifetech ECR8215/F, magnetized agarose-glyoxyl, magnetized fumed silica nanoparticles, silica-coated and polyethilenimine-coated magnetic nanoparticles. Benchmarking among the different supports was conducted taking into account the optimization of several factors such as enzyme retention capacity, loss of enzyme activity during immobilization, ease of the support activation process and cost. Moreover, envisaging the use of immobilized GAO and AAO as a first stage in enzyme cascade synthesis, the biotransformation of 5-HMF was performed and compared with free enzyme.

[O-BB10]

Designing humanized hydrogels toward tissue engineering and disease modeling

C.A. Custódio[1,*], S.S. Santos[1], C.F. Monteiro[1], J.F. Mano[1]
[1] 1- Department of Chemistry, CICECO, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal;
*catarinacustodio@ua.pt



Currently, 3D in vitro cell cultures that lead to more predictive models for research are emerging not only as a new tool in early drug discovery, but also as potential therapeutics to treat disease. For example, basement membrane extracted from the Engelbreth-Holm-Swarm (EHS) mouse sarcoma or collagen matrices have shown to drive cellular self-organization and complex morphogenetic processes to result in sophisticated 3D cell culture platforms. However, drug screening models using this type of materials go against current animal-free approaches for cell culture and restrict clinical compliance. Despite the design flexibility of synthetic alternatives, they are typically expensive and their synthesis can be time consuming. To overcome these drawbacks, we developed a next-generation of cost effective, easy do handle human based materials for 3D cell culture and microtissue development (patented). This innovative product consists in a bioactive platelet-rich plasma derivative precursor (PLMA) that can be cured upon light exposure to form soft materials with tuneable mechanical properties.

[O-BB11]

Valorization of coffee wastes through acidogenic fermentation

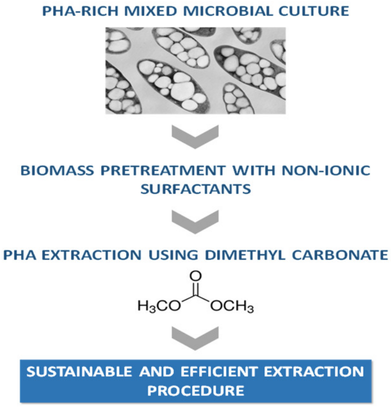
J. Pereira[1,*], *P.C. Lemos*[2], *L.S. Serafim*[1]
[1] *CICECO – Aveiro Institute of Materials, Departamento de Química, Universidade de Aveiro, Aveiro, Portugal;* [2] *LAQV-REQUIMTE, Department of Chemistry, Faculty of Science and Technology, Universidade NOVA de Lisboa. Portugal.*
** joanasofiapereira@ua.pt*

Spent coffee grounds (SCG) are a waste of low value with potential to be valorized into polyhydroxyalkanoates (PHAs). PHAs are bio-based polymers, posing as sustainable alternative to conventional plastics, and can be produced by mixed microbial cultures (MMCs) using wastes or by-products, leading to a significant reduction in the production costs. In this work, the conditions for producing short-chain organic acids (SCOAs), the preferred substrate for PHAs production, from SCGs were evaluated. Different sources of inoculum were studied, and an aerobic MMC showed the best performance. Acidogenic fermentation of SCG using the aerobic inoculum was tested in two reactor configurations, CSTR and FBBR. FBBR showed better results, with a production of 1.53 gSCOAs/L. Pretreatments of SCG were tested, and acid hydrolysis led to the highest increase on SCOAs production. This work showed the potential of SCG valorization via acidogenic fermentation into SCOAs that can be used for PHA production.

[O-BB12]

Non-ionic surfactants as a pretreatment to optimize PHA extraction from mixed microbial cultures

B. Colombo[1], *J. Pereira*[2], *M. Martins*[2], *S. P. M. Ventura*[2], *F. Adani*[1], *L. S. Serafim*[2,*]
[1] *DISAA – Gruppo Ricicla labs - Department of Agricultural and Environmental Sciences - Production, Landscape, Agroenergy, Università degli Studi di Milano, Milan, Italy;* [2] *CICECO – Aveiro Institute of Materials, Departamento de Química, Universidade de Aveiro, Aveiro, Portugal;*
**luisa.serafim@ua.pt.*



Polyhydroxyalkanoates (PHAs) are biodegradable plastics with microbial origin, stored by bacterial cells as granules. PHAs are considered as future substitutes of traditional plastics. However, their application is still limited by their high production costs. In the last years, the possibility of reducing such costs by developing a low-cost PHAs production by mixed microbial cultures using agro-industrial wastes as substrate has been largely explored. However, only few studies were dedicated to the extraction and purification process proved to strongly affect the production costs.

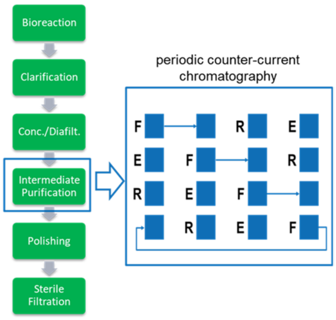
In this work, an alternative PHAs extraction procedure was developed, based on biomass pretreatment with non-ionic surfactants followed by the use of dimethyl carbonate (DMC) as a more sustainable extracting agent. The developed procedure allowed recovering up to 57 % of the polymer content that represents a good result given the heterogeneity of the starting mixed microbial culture.

[O-BB13]

Design of a periodic counter-current chromatography process for efficient oncolytic virus purification

R.J.S. Silva[1*], *J.Mendes*[1], *M.Berg*[2], *.L.Mathiason*[2], *C.Peixoto*[1,3], *P.M. Alves*[1,3],
M.J.T. Carrondo[1]

[1] *iBET - Instituto de Biologia Experimental e Tecnológica, Apartado 12, 2780-901 Oeiras, Portugal;* [2] *GE Healthcare Bio-Sciences AB, Björkgatan 30, 751 84 Uppsala, Sweden;* [3] *Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de Lisboa, Av. da República, 2780-157 Oeiras, Portugal;*
**rsilva@ibet.pt.*



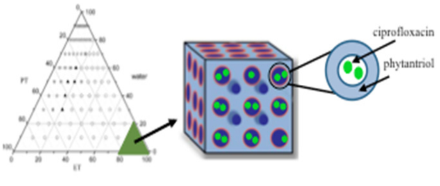
Over the past two decades, biopharmaceutical industry observed a shift in the allocation of manufacturing limiting steps, from upstream to downstream processing. The use of continuous chromatography for biologics presents a way to address the productivity improvement challenges required for debottlenecking downstream operations. Although the adoption of these type of processes is becoming more common in the biopharmaceutical industry, namely for mAbs purification, there is still a long path to fully adopt these technologies as a standard practice in downstream processing.We report on the design of a periodic counter-current chromatography process applied to the intermediate purification of an oncolytic adenovirus.

[O-BB14]

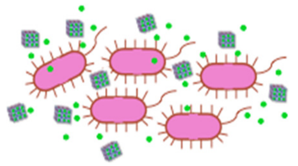
Novel nano-engineering phytantriol-F127-based cubosomes for antibiotic delivery

J. Domingues[1,2*], *M.O. Pereira*[1], *A.M. Sousa*[1,], *B.FB. Silva*[2]

[1] *CEB-Centre of Biological Engineering, LIBRO- Laboratório de Investigação em Biofilmes Rosário Oliveira, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal;* [2]*INL-International Iberian Nanotechnology Laboratory, 4715-330 Braga, Portugal.*
** joana71499@gmail.com*



Cubosomes preparation



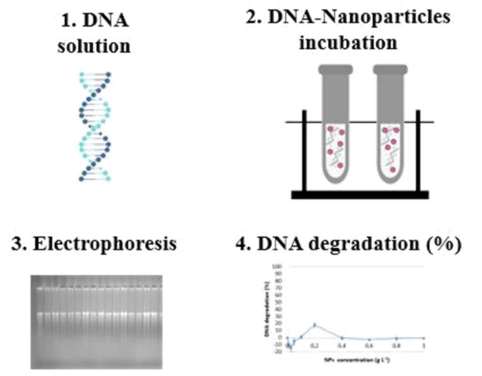
Antimicrobial action of ciprofloxacin-loaded cubosomes

Nanoparticles exhibited exceptional properties for drug delivery via different routes with excellent pharmacokinetics profiles using minimal dosages with almost no systemic side effects. The delivery of drug molecules for therapeutic applications usually faces problems of solubility and bioavailability that cubosomes can easily overcome. Cubosomes are cubic lipid-based nanoparticles with increased surface area, low viscosity and high heat stability. The preparation of cubosomes and drug encapsulation are still procedures requiring important improvements that have limit their use as drug delivery system. This work we developed a simple experimental procedure able to produce controlled-size cubosomes with different hydrodynamic size dependent of the phytantriol/ethanol (lipid/hydrotrope) ratio. Moreover, cubosomes were easily loaded with ciprofloxacin without structural changes. The results of this study will greatly impact on the applicability of cubosomes as drug delivery system.

[O-BB15]

Genotoxicity analysis of different magnetite-based nanoparticles applied in chemical catalysis processes

M. Gamallo[1, *], S. Silva[2], M.E. Pintado[2], G. Feijoo[1], M.T. Moreira[1]
[1] Universidade de Santiago de Compostela, ETSE, Rua Lope Gomez de Marzoa s/n, Santiago de Compostela, Spain;
[2] Universidade Católica Portuguesa/Porto, CBQF, Rua Arquiteto Lobao Vital, Apartado 2511, 4202-401, Porto, Portugal
* maria.gamallo.miron@gmail.com



Eco-toxicity is an important consideration in understanding the potential environmental impacts of the release of nanomaterials into the environment. In this study, the potential genotoxicity of nanosized magnetic iron-based oxide particles used in the treatment of contaminated effluents by chemical catalysis processes such as Fenton reaction or photocatalysis was investigated using a simple method for the quantitative evaluation of DNA degradation. The selected nanoparticles were magnetite (Fe_3O_4), silica, citrate, poly (acrylic acid) and polyethylenimine coated magnetite (Fe_3O_4@SiO_2, Fe_3O_4@Citratete, Fe_3O_4@PAA, Fe_3O_4@PEI) and two different magnetite nanocomposites with TiO_2 and ZnO. The obtained results highlight the need for caution during the use and disposal of these manufactured nanomaterials, as DNA oxidation effects may be observed at very low concentrations.

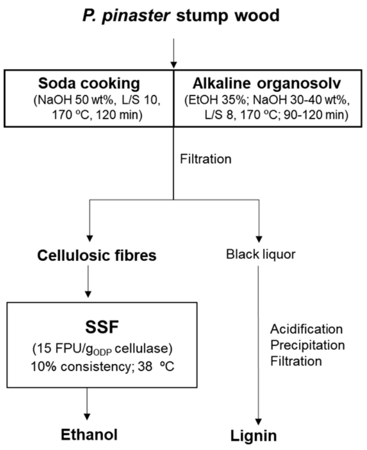
Oral Session

BIOREFINERY AND SUSTAINABILITY

[O-BS01]

Production of ethanol from *Pinus pinaster* stump wood extracted pulp and lignin recovery

*C. Mendes**, *R. Moreira, A. Portugal, M.G. Carvalho*
Chemical Process Engineering and Forest Products Research Centre (CIEPQPF), Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, Portugal;
**catvan@eq.uc.pt*

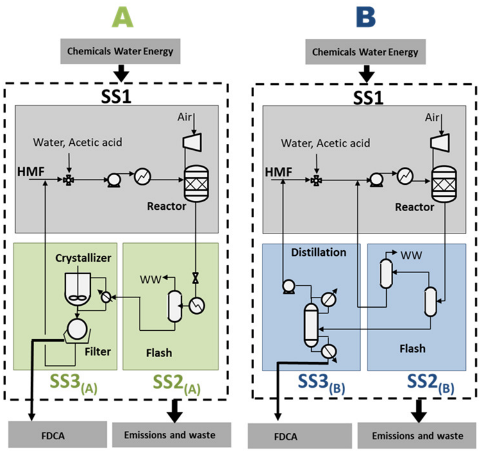


Pinus pinaster stump wood was processed by soda (SA) and alkaline organosolv (AOS) pulpings using different operating conditions. Black liquors of soda and organosolv cooking were acidified in order to precipitate dissolved lignins. Both pulps and precipitated lignins were characterized in terms of hemicelluloses, cellulose and lignin contents. The pulps were further processed by simultaneous saccharification and fermentation (SSF), using 10% pulp consistency, 15 FPU/g$_{ODP}$ of Cellic® CTec2 enzyme and *Saccharomyces cerevisiae* ATCC® 26602™ yeast, to produce bioethanol. An ethanol concentration of 47.0 g/L was produced from SA pulp, with a production rate and ethanol yield of 1.0 g/(L·h) and 89.1%, respectively. The SSF of AOS pulps yielded ethanol concentrations up to 43.9 g/L, with a productivity c.a. 1.6 g/(L·h) and conversion yield up to 88.1%. Ethanol concentration and bioconversion yield decreased with the increase of lignin content in the pulp.

[O-BS02]

Toward the improved sustainability of bioplastics: process modelling and life cycle assessment of an FDCA production route

S. Bello, P. Mendez-Trelles, E. Rodil, G. Feijoo, M.T. Moreira
[1] *Universidade de Santiago de Compostela, ETSE, Rua Lope Gomez de Marzoa s/n, Santiago de Compostela, SPAIN;*
* *sara.bello.ould@gmail.com*

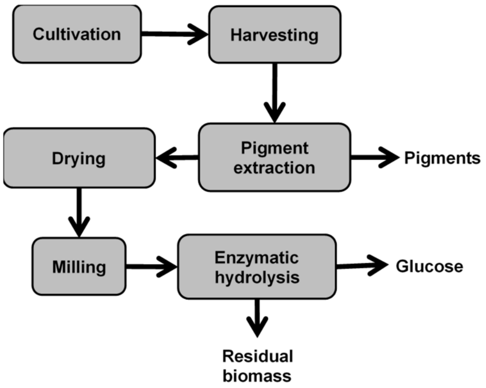


Leading research trends nowadays are geared towards the production of alternatives that compete with fossil-based materials. Issues like the increase of plastic waste or the finite nature of oil make it imperative to study sustainable production routes. Process modelling with Aspen Plus® has allowed to assess the production of 2,5-furandicarboxilic acid (FDCA) from lignocellulosic 5-hydroxymethyl furfural (HMF). FDCA is the precursor of bioplastics such as polyethylene furanoate, which has a great potential to be a direct competitor of polyethylene terephthalate. This study has been focused on the modelling of FDCA synthesis in a catalytic reactor with two different downstream options: A) crystallization, B) distillation. When dealing with renewable feedstocks, one of the most relevant challenges is to guarantee their sustainability. Thus, life cycle assessment has allowed to pinpoint the processing areas with most environmental burden: the production of HMF and the energy consumption.

[O-BS03]

Biorefinery approach for obtaining pigments, sugars and a protein-rich residue from microalgae

M.F. Souza[1,*], *M.A. Rodrigues*[2], *E.P.S.Bon*[2], *S.P. Freitas*[1]
[1] *Federal University of Rio de Janeiro, School of Chemistry, Av Athos da Silveira Ramos, Rio de Janeiro, Brazil;* [2] *Federal University of Rio de Janeiro, Chemistry Institute, Av Athos da Silveira Ramos, Rio de Janeiro, Brazil*
[*] *cellafsouza@gmail.com*

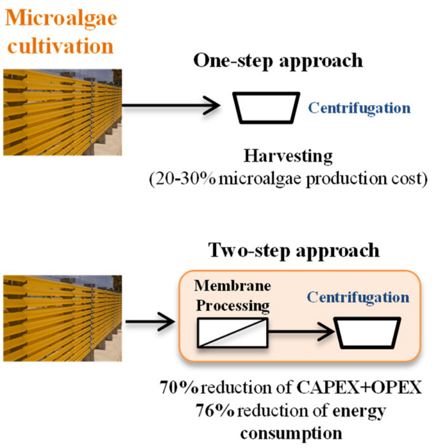


The aim of this work was to evaluate the starch accumulation in the microalga *Chlorella sorokiniana* and process its whole biomass in a biorefinery approach. Nitrogen starvation triggered starch accumulation in *C. sorokiniana*, resulting in a maximum starch content of 26% (w/w). The starch-rich biomass was harvested by sedimentation and the fresh cells were subjected to a treatment with ethanol in order to extract pigments prior to the hydrolysis step. After the extraction, the ethanol impregnated cells were more easily dried than the fresh cells, reducing the energy requirements of the drying step. Extracted dried cells were then milled for cell wall disruption, resulting in a biomass highly susceptible to hydrolysis with amylases, with glucose yields higher than 90% within 4 hours of processing. The resulting hydrolyzed biomass is rich in proteins and lipids and could be used for human or animal nutrition.

[O-BS04]

Harvesting of carotenogenic phase *Dunaliella salina* by membrane filtration at lab and pilot scale

J. Monte[1,*], *J. Bernardo*[1], *M. Sá*[1], *C.F. Galinha*[1], *L. Costa*[2], *C. Casanovas*[3], *C. Brazinha*[1], *J.G. Crespo*[1]
[1] *LAQV-REQUIMTE, Chemistry Department, FCT, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal;* [2] *A4F – Algae for Future, Campus do Lumiar, Estrada do Paço do Lumiar, Edif. E, R/C, 1649-038 Lisboa, Portugal;* [3] *Monzón Biotech, Baldiri Reixach, 4-12 y 15 - 08028, Barcelona, Spain*
** joana_monte@campus.fct.unl.pt*

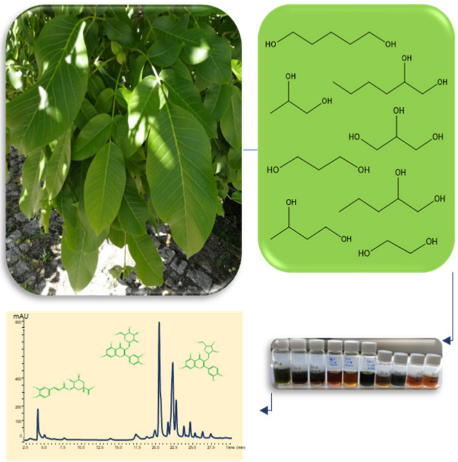


Dunaliella salina is an unicellular microalga, well-known for its high content in carotenoids, especially β-carotene. This microalgae is very fragile and shear sensitive due to lack of rigid cell wall. Therefore, it can easily rupture when excessive shear stress is applied. This work aims to investigate the potential of pre-concentrating *D. salina* by membrane processing prior a final step of centrifugation. The aim is to minimise the overall energy and capital costs, while assuring a low percentage of loss of integrity and high permeate fluxes. The harvesting process was performed under controlled permeate fluxes at lab and pilot scale. At pilot scale, harvesting of *D. salina* by ultrafiltration allowed reaching a final concentration factor of 10, with an average permeate flux of 21 L/m^2.h. The Total Cost of Ownership and energy consumption were respectively 70% and 76% lower, when applying a two-step approach of a membrane-centrifugation system compared to solely centrifugation.

[O-BS05]

Polyols: efficient solvents to extract phenolic compounds from walnut leaves

V. Vieira[1-3]*, A. Feitor*[2]*, M.A. Prieto*[2,4]*, R. Calhelha*[2]*, L. Barros*[2,3]*, J.A.P. Coutinho*[2]*, O. Ferreira*[2,3*]*, I.C.F.R. Ferreira*[2,*]
[1]*Aveiro Institute of Materials (CICECO), University of Aveiro, Complexo de Laboratórios Tecnológicos, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal;* [2]*Mountain Research Centre (CIMO), Campus de Santa Apolónia, 5300-253 Bragança, Portugal;* [3]*Associate Laboratory LSRE-LCM, Campus de Santa Apolónia, 5300-253 Bragança, Portugal;* [4]*Nutrition and Bromatology Group, Faculty of Food Science and Technology, University of Vigo, Ourense Campus, E32004 Ourense, Spain.*
** iferreira@ipb.pt ; oferreira@ipb.pt*

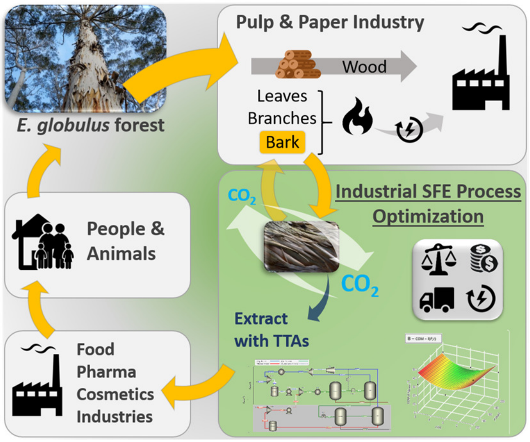


In this work, a set of polyols was studied to extract phenolic acids and flavonols from walnut leaves (*Juglans regia*), a rich source of bioactive phenolic compounds. The solvent screening included glycerol and a series of diols (1,2-ethanediol, 1,2-propanediol, 1,3-propanediol, 1,3-butanediol, 1,2-pentanediol, 1,5-pentanediol, 1,2-hexanediol, 1,6-hexanediol). The extraction yield was quantified and the bioactivity of the extracts was evaluated by measuring the antioxidant, cytotoxic and anti-inflammatory activities. The best combined results were obtained with 1,2-propanediol and 1,3-propanediol. The extraction yields were similar to the results obtained with ethanol. Moreover, those extracts do not present cytotoxicity for non-tumor cells (PLP2) and reveal significantly higher antioxidant activity and cytotoxicity for a tumor cell line (HeLa) when compared to the aqueous extract. The results obtained provide relevant information regarding the use of alternative solvents that could potentially be used as formulation media in the pharmaceutical or cosmetics areas.

[O-BS06]

Supercritical CO_2 extraction of *Eucalyptus globulus* bark: Techno-economic optimization of the industrial process

V.H. Rodrigues, M.M.R. de Melo, I. Portugal, C.M. Silva*
Department of Chemistry, CICECO – Aveiro Institute of Materials, University of Aveiro,
Campus Universitário de Santiago 3810-193, Aveiro, Portugal
** vitorhrodrigues@ua.pt*

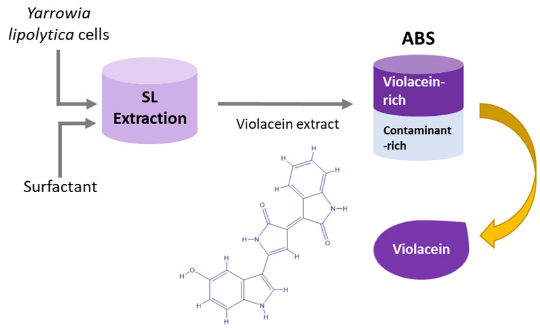


This work aimed the design and simulation of an industrial scale process of supercritical fluid extraction (SFE) of *E. globulus* bark, as well as the techno-economic optimization for different process responses: Total Yield, Cost of Manufacturing (COM), Productivity and Process Energy. An extensive matrix of SFE datapoints was prepared, including new simulated extraction curves produced using Broken plus Intact Cells modeling. Then, an experimental optimization was applied to five operating conditions: pressure (120 – 200 bar), temperature (40 – 60 ^{0}C), cosolvent (ethanol) content (0 – 5 wt.%), solvent (CO_2) flow rate (6 – 12 g min^{-1}) and extraction time (1, 3 and 5 h). The optimal results scored 1.15 wt.% for Total Yield, 28.1 € $kg^{-1}_{extract}$ for COM, 364 $ton_{extract}$ $year^{-1}$ for Productivity, and 0.436 GJ $kg^{-1}_{extract}$ for Process Energy. The present study provides strong techno-economic arguments towards the investment in SFE technology for the valorization of *E. globulus* bark.

[O-BS07]

Aqueous solutions of surface-active agents on the recovery of violacein from *Yarrowia lipolytica* cells

M. Kholany[1,], J. Vieira[1], M. Martins[1], S.P.M. Ventura[1], P. Trébulle[2], J. Nicaud[2], J.A.P. Coutinho[1]*
[1]CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal; [2]Micalis Institute, INRA, AgroParisTech, Université Paris-Saclay, 78350 Jouy-en-Josas, France.
** mariamkholany@ua.pt*

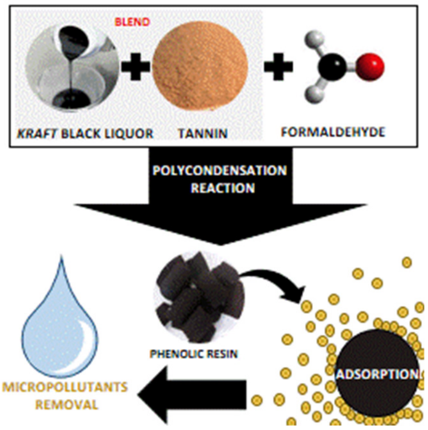


The focus of this work is to optimize the extraction and purification of a purple-blue pigment - violacein, with appealing biological activities. With this aim, a large array of tensioactive agents was tested in solid-liquid extraction processes. Furthermore, some operational conditions, such as the solid-liquid ratio, the effect of consecutive extractions, the time of extraction and the concentration of the solvent were evaluated. Once the optimized extract was attained, the application of purification systems was pursued. Aqueous biphasic systems (ABS) composed of surfactant and cholinium-based ionic liquids (ILs) were characterized and applied in the purification of violacein from the remaining cellular contaminants, namely proteins. Thus, the development of an integrated process for the recovery of this biomolecule was achieved with success and in a sustainable way.

[O-BS08]

Sustainable phenolic resin: a potential adsorbent for amoxicillin removal

W.M. Moreira[1,], P.V. Viotti[1], C.M.S.G. Baptista[2], M.H.N.O. Scaliante[1,*], M.L. Gimenes[1]*
[1] State University of Maringá, Av. Colombo, 5790 – Jardim Universitário, Maringá, Paraná, Brazil; [2] CIEPQPF - Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, R. Sílvio Lima, Polo II, 3030-790 Coimbra, Portugal.
** wardleison@gmail.com*

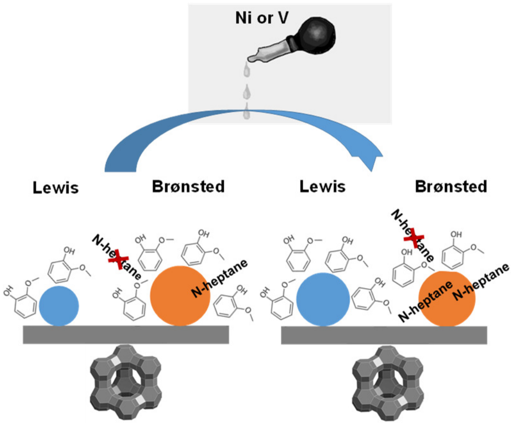


Micropollutants are an emerging problem as they affect the health and quality of life of humans and aquatic environment. In this scenario, the adsorption process emerges as a promising alternative for water decontamination. The present work evaluated the use of a phenolic resin as a potential adsorbent for amoxicillin removal from wastewater. The sustainable phenolic resin was synthetized by reaction of formaldehyde with a blend of *Kraft* black liquor and tannin, used as alternative precursors of phenolic compounds. The textural and structural evaluation indicated the low specific surface area of the resin and a great variety of surface functional groups. Phenolic resin exhibited promising results as an adsorbent for amoxicillin removal. For comparison purpose, the adsorption was also conducted by replacing the resin by activated carbon. The adsorption onto phenolic resin occurred at higher rates and the equilibrium was achieved after 8 hours, with a removal of 60%.

[O-BS09]

FCC feedstocks/bio-oils co-processing: Towards understanding of phenolic compounds impact on Ni- and V-USY zeolites

R. T. Jacob Gerards[1], *Inês Graça*[2], *M. Filipa Ribeiro*[1*]
[1] *CQE-Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais 1, 1049 – 001 Lisboa, Portugal;* [2] *Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK*
**filipa.ribeiro@tecnico.ulisboa.pt.*



An option to produce second generation bio-fuels could consist of co-feeding hydrotreated bio-oils with traditional Fluid Catalytic Cracking (FCC) feedstocks. A key aspect of this co-processing is the presence of phenolic compounds, which have a detrimental impact on the acidic zeolites in FCC catalysts. However, metal contamination by Ni and V species present in the feedstock also takes place during the process, which might influence this deactivating effect. Thus, catalytic tests were performed with a model hydrocarbon (n-heptane) and a model bio-oil derived molecule (guaiacol) at 450ºC, on Ni- and V-USY zeolites. The deactivating effect of guaiacol was observed to be partially attenuated with V and fully suppressed by Ni at 2% incorporation, owing to the Lewis acidity increase upon metal impregnation, especially for Ni. As a result, guaiacol molecules will preferentially adsorb on the Lewis acid sites, protecting the Brønsted acidity responsible for the cracking reactions.

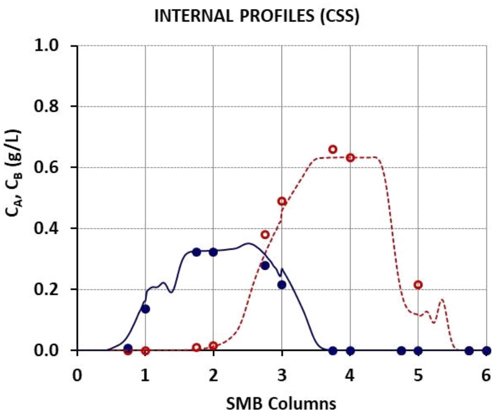
Oral Session

REACTION AND SEPARATION PROCESS

[O-RS01]

Separation of nadolol racemates by high pH reversed-phase simulated moving bed chromatography

R. Arafah[1,2], A. Ribeiro[1,2], A. Rodrigues[2], L. Pais,[1,2,]*
[1]Centro de Investigação de Montanha (CIMO), Polytechnic Institute of Bragança, Campus de Santa Apolónia, Apartado 1134, 5301-857 Bragança, Portugal; [2]Laboratory of Separation and Reaction Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal.
** pais@ipb.pt*

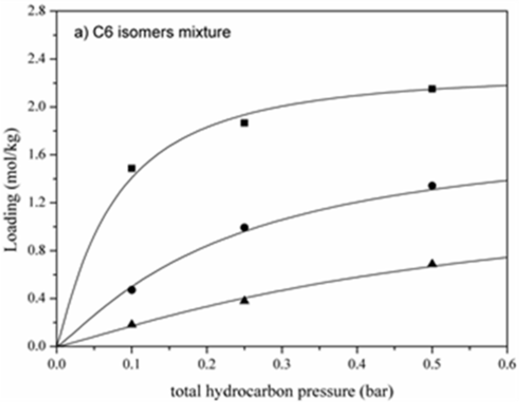


Nadolol is a pharmaceutical drug marketed as a mixture of four stereoisomers, used to treat cardiovascular diseases. This drug is a mixture of two pairs of racemates, therefore, its complete separation represents a challenging task. Recently, our research group reported the pseudo-binary separation of nadolol by SMB chromatography using both coated Chiralpak AD and Chiralpak IA immobilized chiral stationary phases. In this work, we present an alternative strategy, implementing a first achiral separation step, by using C18 columns to perform the separation of the two pairs of nadolol racemates under reversed-phase mode. Extensive experimental and simulation results will be presented including solvent screening, measurement of equilibrium and kinetic data, and both fixed-bed and SMB preparative separations. Extensive experimental and simulation results will be presented, including solvent screening, measurement of equilibrium adsorption isotherms, breakthrough measurements, and SMB (FlexSMB-LSRE unit) experimental preparative separation using C18 columns.

[O-RS02]

Separation of hexane isomers in metal organic framework ZIF-8

A. Henrique[1,2], M. Karimi[1,2], P. Brântuas[1,2], J.A.C. Silva[1,2], A.E. Rodrigues[1]*
1 Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Faculdade de Engenharia da Universidade do Porto, Porto, Portugal; 2 Sustainable Processes and Products Group, Mountain Research Center (CIMO), Instituto Politécnico de Bragança, Bragança, Portugal;
**adriano_henrique@ipb.pt.*

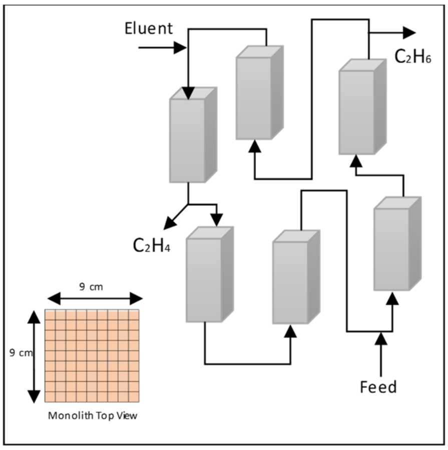


The performance of porous metal organic framework ZIF-8 in the separation of all five hexane isomers (nHEX, 2MP, 3MP, 23DMB, 22DMB), is evaluated through a series of multicomponent breakthrough adsorption experiments, at the temperatures of 373, 423 and 473 K and up to partial pressures of 0.5 bars. The reported data shows for all experiments the following sorption hierarchy: nHEX >> 2MP > 3MP >> 23DMB > 22DMB. It is also demonstrated that the sorption of nHEX is equilibrium based in contrast with the sorption of branched isomers which is kinetic controlled. The experimental data is also simulated through a mathematical model developed in MATLAB code, being the results in qualitatively agreement. This paper shows that it possible to separate the hexane isomers in ZIF-8 by classes linear/mono-branched/di-branched if proper experimental conditions are set-up, being the result of importance for the octane upgrading of gasoline.

[O-RS03]

Ethylene/ethane separation by gas-phase SMB in binderless Zeolite 13X monoliths

R. Seabra[1,], V.F.D. Martins, K. Gleichmann[2], A.M. Ribeiro[1], A.F.P. Ferreira[1], A.E. Rodrigues[1]*
[1]LSRE-Laboratory of Separation and Reaction Engineering, Associate Laboratory LSRE/LCM, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal; [2]Chemiewerk Bad Köstritz GmbH, Heinrichshall 2, 07586 Bad Köstritz, Germany
**ruteseabra@fe.up.pt*

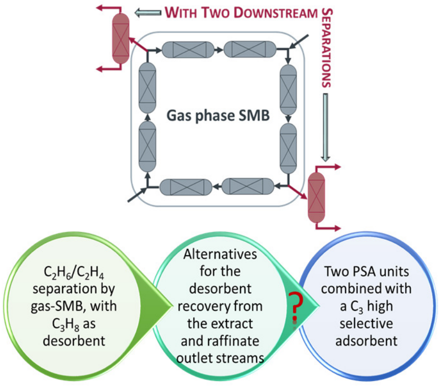


In this work binderless zeolite 13X monoliths were tested as a new promising material for high purity ethylene production from olefin/paraffin mixtures by gas-SMB technology. In order to characterize the adsorbent and its potential for the target separation, the equilibrium isotherms of ethane, ethylene and propane were measured gravimetrically, in a temperature range from 323 K to 423 K, and pressure up to 6 bar. Dynamic studies were performed at 373 K and 1.5 bar in the gas-SMB bench scale unit. For the experiment with 0.48/0.52 ethane/ethylene feed composition, the adsorbent under evaluation was obtained an ethylene purity of 97.7%, with recovery and productivity of 98.0 % and 16.6 $kg_{C2H4} \cdot h^{-1} \cdot m_{bed}^{-3}$, repectively. This work experimentally demonstrated that the gas-phase SMB can be an efficient technology for olefin/paraffin separations and that it is possible to produce high purity grade ethylene with a high recovery using binderless zeolite 13X monoliths as adsorbent and propane as desorbent.

[O-RS04]

An alternative method for the separation of C2/C3 hydrocarbons mixtures by pressure swing adsorption using the MOF MIL-100(Fe)

V.F.D. Martins[1], R. Seabra[1], P. Silva[1], A.M. Ribeiro[1], J.-S. Chang[2,3], J.M. Loureiro[1], A. Ferreira[1,], A.E. Rodrigues[1]*
[1] Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Department of Chemical Engineering, University of Porto, Rua Dr. Roberto Frias, s/n, 4200-465, Porto, Portugal; [2] Catalysis Center for Molecular Engineering, Korea Research Institute of Chemical Technology (KRICT), Jang-dong 100, Yuseong, Daejeon, Republic of Korea; [3] Department of Chemistry, Sungkyunkwan University, Suwon 440-476, Seoul, Republic of Korea.
** aferreir@fe.up.pt*

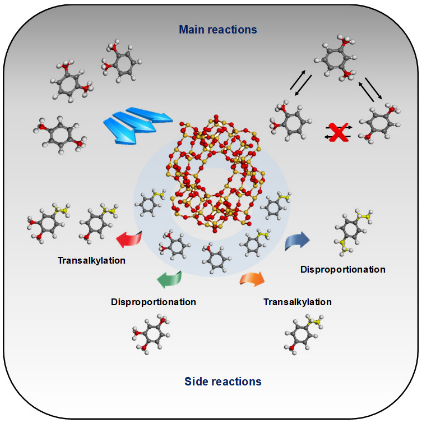


The main objective of this work is the separation of 0.30/0.70 ethane/propane and 0.30/0.70 ethylene/propane, representative mixtures of the outlet streams of the ethane/ethylene separation by gas-phase SMB, using propane as desorbent. Since adsorption equilibrium data are essential for the process design, the adsorption isotherms of ethane, ethylene and propane were measured at 323, 373 and 419 K by a gravimetric method. Fixed-bed experiments were conducted at 0.5 SLPM, 323 K and 150 kPa feed conditions on a lab-scale VPSA unit to obtain fundamental information for the process modelling. Two five-steps VPSA cycles were designed using gProms software and performed experimentally. The performance parameters demonstrated the high viability of the proposed processes, since ethane and ethylene were obtained at high purities (99.9%), with a recovery of 76.2% and 63.9%, respectively.

[O-RS05]

Simulated moving bed reactor for the production of *p*-xylene: isomerization, disproportionation and transalkylation reactions of xylene isomers, ethylbenzene, and toluene in liquid phase

Q. Shi[1], *J.C. Gonçalves*[1*], *A.F.P. Ferreira*[1], *M.G. Plaza*[2], *A.E. Rodrigues*[1]
[1] Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, s/n, 4200-465 Porto, Portugal.
[2] Energy Processes and Emissions Reduction Group (PrEM), Departament of Coal, Energy and Environment, Instituto Nacional del Carbon (INCAR), Consejo Superior de Investigaciones Científicas (CSIC), C/Francisco Pintado Fe 26, 33011, Oviedo, Spain.
** jcgs@fe.up.pt*

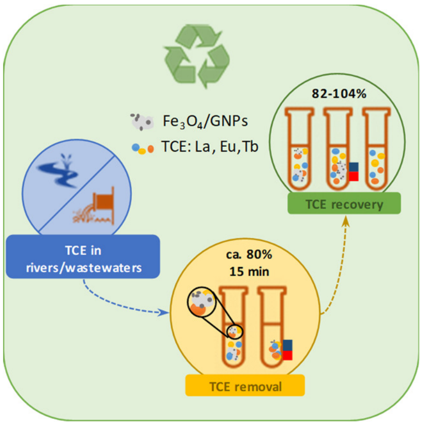


An experimental and parametric behavior study, of xylene isomerization and the considered main side reactions that may occur in a Simulated Moving Bed Reactor (SMBR) for the production of *p*-xylene, was conducted in liquid phase, over beta zeolite. Different reaction schemes were investigated; the linear reaction scheme, taking into account the thermodynamic equilibrium, proved to be the best representation for the isomerization of xylenes. By conducting mixture experiments of the C_8 isomers with and without toluene, ethylbenzene disproportionation and ethylbenzene-toluene transalkylation were identified as the main side reactions in the studied conditions. Both reactions were confirmed to be second order following the deethylation-ethylation mechanism; similar values obtained from pure ethylbenzene and ethylbenzene-toluene experiments indicated the absence of competition between the two reactions. Kinetic parameters and activation energies were obtained for all reactions studied.

[O-RS06]

Removal and recovery of technology-critical elements from aqueous solutions using Fe_3O_4/graphite nanoplatelets

E.L. Afonso[1], *L. Carvalho*[2], *C. Vale*[3], *E. Pereira*[4], *C.M. Silva*[1], *T. Trindade*[1], *C.B. Lopes*[1,3,*]
[1] CICECO, University of Aveiro, 3810-193 Aveiro, Portugal; [2] Central Laboratory of Analysis, University of Aveiro, 3810-193 Aveiro, Portugal; [3] CIIMAR, 4450-208 Matosinhos, Portugal; [4] CESAM, University of Aveiro, 3810-193 Aveiro, Portugal;
** claudia.b.lopes@ua.pt*

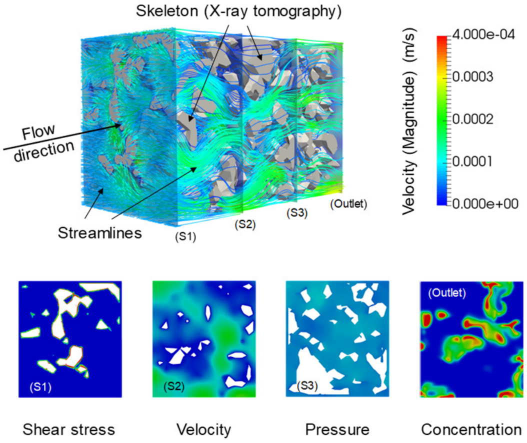


Magnetic graphite-like nanoplatelets (Fe_3O_4/GNPs) were successfully prepared by the electrostatic assembly of graphite nanoplatelets and magnetite nanoparticles. Their potential as sorbent for the removal of technology-critical elements was investigated. The Fe_3O_4/GNPs exhibited good sorption properties towards trivalent lanthanides (La, Eu and Tb). The sorption process is sensitive to solution pH and to the amount of sorbent used. Removal efficiencies up to 80% were achieved using alkaline solutions (pH 8) and 50 mg/L of sorbent. In ternary model solutions, Fe_3O_4/GNPs showed preferential removal for Eu and Tb. The kinetic is well fitted by the pseudo second-order kinetic model, and the equilibrium evidenced a rare but interesting behaviour well depicted by the isotherm measured. At low equilibrium solution concentrations, the system is approximately irreversibly but becomes essentially vertical as the concentration increases. The composite can be reused without loss of efficiency.

[O-RS07]

CFD modelling of flow patterns, tortuosity and residence time distribution in monolithic porous columns reconstructed from X-ray tomography data

S. Pawlowski[1,], N. Nayak[1,2], M. Meireles[2,*], C.A.M. Portugal[1], S. Velizarov[1], J.G. Crespo[1]*
[1] LAQV-REQUIMTE, DQ, FCT, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal; [2] LGC, Université de Toulouse, CNRS, F-31062 Toulouse, France.
** s.pawlowski@fct.unl.pt*

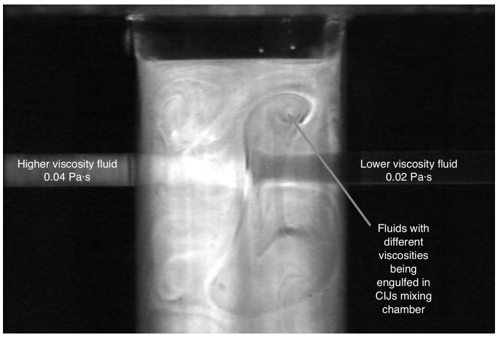


In this work, the morphological structure of a monolith was reconstructed using 3D X-ray tomography data. Subsequently, OpenFOAM CFD package was used to simulate the essential parameters for monoliths' performance characterization such as velocity and pressure fields, streamlines, shear stress and residence time distribution (RTD). Moreover, the tortuosity was directly assessed by measuring lengths of the streamlines which, in laminar regime and steady state, represent the fluid pathways.It was observed (for the case of the monolith studied) that fluid transport was dominated by flow heterogeneities and advection, while the shear stress at pore mouths was significantly higher than in other regions, which is especially important in protein separations. The proposed modelling approach was successfully validated by an experimentally obtained RTD.The herein presented CFD modelling approach can be used to optimise and virtually test the performance of chromatographic materials before being printed/manufactured, thus leading to production of target materials.

[O-RS08]

Mixing of dissimilar fluids in confined impinging jets – Mayonnaise equation

*M. S. C. A. Brito[1], C.P. Fonte[2], M. M. Dias[1], J. C. B. Lopes[1], R. J. Santos[1]**
[1] Associate Laboratory LSRE-LCM, Faculdade de Engenharia da Universidade do Porto, Rua do Dr. Roberto Frias, 4200-465 Porto, Portugal; [2] School of Chemical Engineering and Analytical Science, The University of Manchester, Oxford Road, Manchester M13 9PL, U.K.
**rsantos@fe.up.pt*

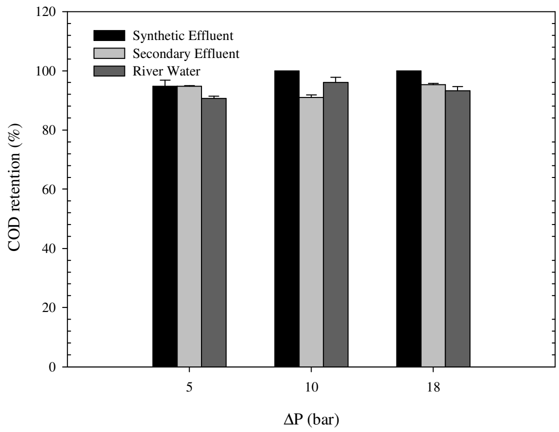


CIJs can efficiently mix fluids with different viscosities at non-unitary flow rate ratios. In this communication it is presented the experimental and numerical characterization of the flow in CIJs for fluids with a viscosity ratio of 1:2. Experimental characterization is made with Planar Laser Induced Fluorescence, and numerical study is based on 3D CFD simulations of CIJs. Experimental and numerical results show that the balance of kinetic energy rate of the opposed jets plays the key role on the jets impingement point positioning, although viscosity also has an impact on this. Mayonnaise equation, previously introduced, makes a good prediction of the best CIJS design to effectively mix dissimilar fluids.

[O-RS09]

Removal of the mixture of pharmaceuticals sulfamethoxazole and diclofenac from water streams by a polyamide nanofiltration membrane

*D.S. Gomes, M. Cardoso, R.C. Martins, R.M. Quinta-Ferreira, L.M. Gando-Ferreira**
CIEPQPF – Chemical Processes Engineering and Forest Products Research Center, Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, Pólo II – Rua Sílvio Lima, 3030-790 Coimbra, Portugal.
** lferreira@eq.uc.pt*

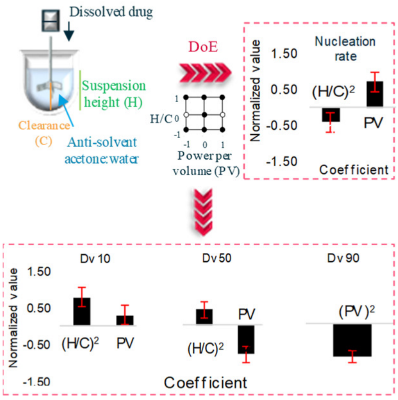


This work aims to investigate and optimize the performance of the Trisep TS80 nanofiltration (NF) membrane for the removal of a mixture of two most detected pharmaceutical compounds in municipal wastewaters worldwide, Sulfamethoxazole (SMX) and Diclofenac (DCF). Several NF tests were carried out to study the rejections of these contaminants spiked both in demineralized water, filtrated natural water and secondary effluent. pH was the variable that most affected the contaminants rejection and membrane permeability. In the case of synthetic effluent, an applied pressure of 10 bar and pH 7 were determined as the best operating conditions, which allowed achieving almost total COD retention and a global contaminants rejection of 96.3%. The application of different water matrices (river water and secondary municipal effluent) had no significant impact on process efficiency. *Vibrio fischeri* luminescence inhibition tests revealed that treatment by nanofiltration reduced acute toxicity of all studied effluents.

[O-RS10]

Assessment of the influence of clearance and agitation on the nucleation rate and particle size distribution in anti-solvent crystallization process of a drug substance

A. Tulcidas[1,2,], B. Santos[2], S. Pawlowski[3], F. Rocha[1]*
[1]Faculty of Engineering University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal; [2]Hovione Farmaciência SA, Rua Comandante Carvalho Araújo, 2674-506 Loures, Portugal; [3] NOVA University of Lisbon, 2829-516 Caparica, Portugal.
** ameessa.tulcidas@gmail.com*

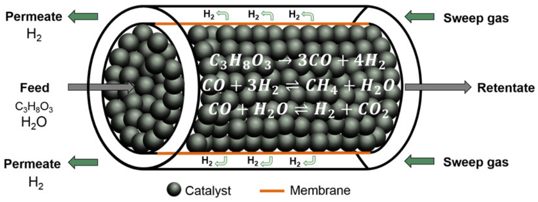


The impact of reactor hydrodynamics on the nucleation rate and Particle Size Distribution (PSD) of a drug substance produced in an anti-solvent crystallization process was evaluated. For this purpose, a Design of Experiment (DoE) approach was employed, where the suspension height:clearance ratio and power per volume were varied along the crystallization. Subsequently, in order to better understand the interaction among the variables, correlations were found by Multiple Linear Regression (MLR). It was found that both nucleation rate and the particle size distribution can be influenced by the suspension height:clearance (H/C) ratio and power per volume (PV). The nucleation rate seems to increase when the ratio decreases and increases when the power per volume increases. Larger particles seem to be produced when a higher ratio and lower power per volume are employed.

[O-RS11]

Glycerol steam reforming for hydrogen production: traditional *versus* membrane reactor

*M.S. Macedo, M.A. Soria, L.M. Madeira**
LEPABE, Department of Chemical Engineering, Faculty of Engineering, University of Porto
Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal
* *mmadeira@fe.up.pt*

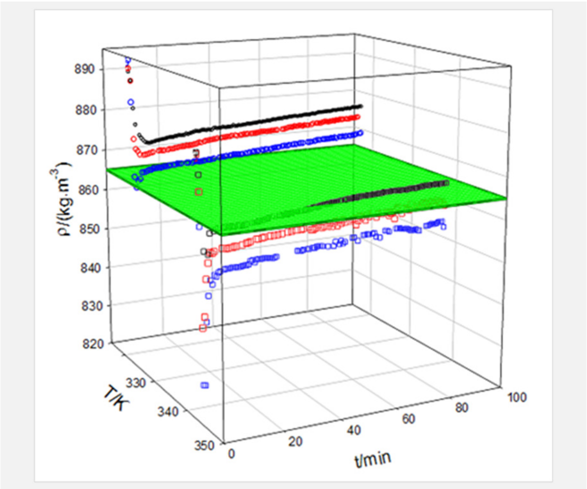


A phenomenological model was developed for predicting the performance of a traditional reactor (TR) versus a membrane reactor (MR) for hydrogen production via glycerol steam reforming (GSR). A parametric analysis was carried out for different ranges of conditions, namely: temperatures of 773-973 K for the TR and 673-773 K for the MR (due to restrictions of existing Pd-based H_2 permselective membranes), water-to-glycerol feed ratios (WGFRs) of 4-12 and total pressures of 100-500 kPa; the membrane thickness influence in the MR was also assessed. For the same operating conditions (773 K, WGFR of 4 and 500 kPa), the MR showed an enhancement in the H_2 yield over 220 % when compared with the TR. Finally, when the maximum amount of H_2 production was analyzed for both reactor configurations, an increase of 6 % was observed in the MR while allowing reducing the operating

[O-RS12]

Monitoring the transesterification reaction by continuous off-line density measurements

N.M.C.T. Prieto[1,2], *A.G.M. Ferreirra*[1,*], *A.T.G. Portugal*[1], *R.J. Moreira*[1]
[1] *CIEPQPF, Department of Chemical Engineering, University of Coimbra, Polo II, Rua Silvio Lima, 3030-970 Coimbra, Portugal;* *[2] *CECOAL-CONICET-UNNE, Ruta 5 Km 2.5, 3400 Corrientes, Argentina;*
**abel@eq.uc.pt*

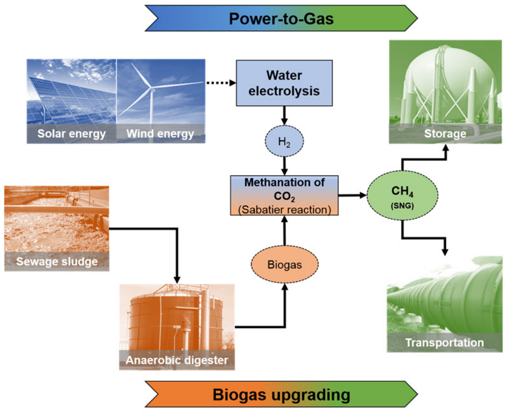


The continuously monitoring of transesterification reaction in industrial production is of high relevance in order to avoid operational problems, eliminate batch sampling and analysis delay and guarantee the quality of the final product through a process control system. Also it is essential for kinetic studies. In this work, the transesterification of cottonseed oil at 50 ºC and 70 ºC, with methanol/oil molar ratios of 4.5, 6.0 and 7.5 were carried out and the oil conversion as a function of reaction time was evaluated by ^1H NMR. The density of the reaction mixture, at these experimental conditions, was measured as a function of the reaction time by an off-line methodology. From the density-time and FAME conversion-time profiles the operative relationships between conversion, density, alcohol to oil ratio and temperature were established. A very good correlation was obtained.

[O-RS13]

Multifunctional reactors for biogas upgrading through CO_2 methanation: thermodynamic considerations

A.C. Faria, C.V. Miguel, L.M. Madeira[1,*]
[1] *LEPABE, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal.*
**mmadeira@fe.up.pt*

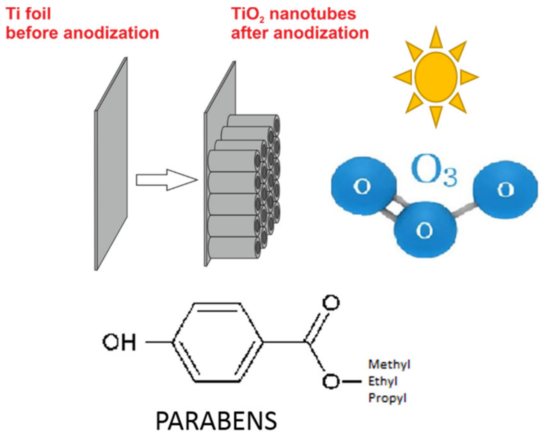


Prior to injection into the natural gas grid or use as vehicle fuel, biogas must undergo an upgrading process for CH_4 purification whereby, globally, the CO_2 is commonly removed by pressure swing adsorption and thereafter emitted to the atmosphere. This work studies an alternative, considering the conversion of CO_2 present in the raw biogas into more CH_4 using renewable-based H_2. The feasibility of such process was assessed thermodynamically, focusing on the Sabatier reaction taking place in the presence or absence of water separation in relevant temperature, pressure and biogas composition ranges. The results showed that the CH_4 yield increases, but only up to an optimum water removal fraction; above this value, coke formation is favored. Still, considering water removal represents a minor impact on CH_4 production, but can be particularly useful to minimize the production of CO_X, allowing to fulfill with the biogas quality specifications for injection into the natural gas grid.

[O-RS14]

Effect of TiO_2 plate supported nanotubes on the solar photocatalytic oxidation and ozonation of parabens mixtures

J. Gomes[1,*], *J. Lincho*[1], *M. Gmurek*[2], *P. Mazierski*[3], *A. Zaleska-Medynska*[3], *R. Quinta-Ferreira*[1], *R. Martins*[1]
[1]*CIEPQPF – Chemical Engineering Processes and Forest Products Research Center, Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, Rua Sílvio Lima, 3030-790 Coimbra, Portugal.* [2] *Faculty of Process and Environmental Engineering, Department of Bioprocess Engineering Lodz University of Technology, Wolczanska 213, 90-924 Lodz, Poland.* [3] *Faculty of Chemistry, Department of Environmental Technology, University of Gdansk, ul. Wita Stwosza 63, 80-308 Gdańsk. Poland.*
** jgomes@eq.uc.pt*



TiO_2 nanotubes supported on titanium foils has been tested for photocatalytic degradation. This kind of approach can be a very suitable option for emerging contaminants degradation considering the possibility of reuse and recover of the catalyst comparing to the case where catalytic powder is used. In this study, besides photocatalytic degradation with sun and UVA radiation also ozonation and photocatalytic ozonation were tested on the degradation of a mixture of three parabens. Ozone coupled with the plates prepared at 20 and 40V improves the single ozonation allowing a reduction on the amount of ozone required for total parabens removal. The UVA radiation with the TiO_2 nanotubes does not promote significant degradation. On the other hand, sunlight radiation for the same plates enhanced the parabens degradation comparing with photolysis. Also catalytic ozonation with the same plates aided by sunlight radiation was tested for the abatement of the parabens mixture.

[O-RS16]

Acidic aqueous biphasic systems: a new paradigm for the ‘one-pot’ extraction of critical metals

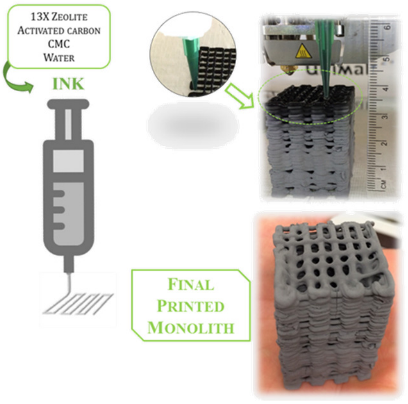
N. Schaeffer[1]*, M. Gras[2], H. Passos[1], V. Mogilireddy[2], I. Billard[2], N. Papaiconomou[2], J.A.P. Coutinho[1]
[1] CICECO, Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.; [2] LEPMI - Universite Grenoble-Alpes, F-38000 Grenoble, France.
* nicolas.schaeffer@ua.pt

Herein, acidic aqueous biphasic system (AcABS) based on ionic liquids (ILs) is proposed as a new extraction-separation platform for the integrated hydrometallurgical treatment of critical metals. AcABS, in which the inorganic salt component of traditional aqueous biphasic system (ABS) is replaced by the acid from the leaching solution, is shown to selectively separate cobalt from nickel, a separation relevant to the recycling of NiMH batteries. Selective electrodeposition of cobalt directly from IL rich phase was optimised based on the partition of the different system components, namely Cl^- and H_3O^+ as well as water content. Selective deposition of cobalt in the presence of co-extracted manganese impurities was achieved in various AcABS derived systems resulting in highly tailored cobalt deposits. These results highlight the potential of AcABS derived systems as a ‘one-pot’ approach for metal treatment from leaching to electrodeposition.

[O-RS17]

Electrical conductive 3D printed monolith adsorbent for CO_2 capture applications

M.J. Regufe*, A.F.P. Ferreira, J.M. Loureiro, A.E. Rodrigues, A.M. Ribeiro
LSRE-Laboratory of Separation and Reaction Engineering, Associate Laboratory LSRE/LCM, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal
* mjregufe@fe.up.pt

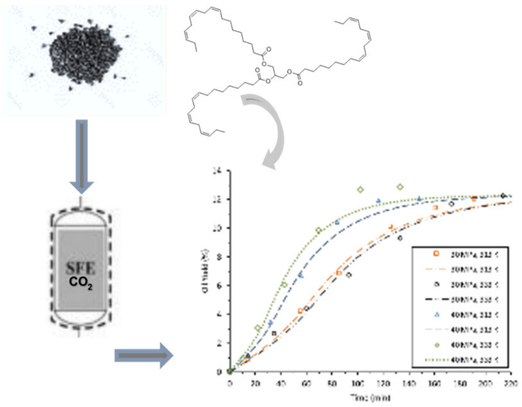


The development of an adsorbent material by 3D printing technology with high CO_2 adsorption capacity and electrical conductivity is presented for application in Electric Swing Adsorption process. The adsorbent is composed by 13X zeolite, activated carbon and binder. The prepared ink was characterized in order to determine the rheological properties of the mixture. The monolith was printed with 30×30×43 mm of dimensions. Textural characterization was performed by diverse techniques, including CO_2 adsorption isotherm at 273 K measurement, being expected that the 3D printed monolith would have high CO_2 adsorption capacity. Heating of material was tested by Joule effect through an electric current passage in the monolith. An increase of temperature of about 80 K during 180 s was verified with a power consumption of 3.25 W, demonstrating that the printed material is suitable for ESA processes applied for CO_2 capture.

[O-RS18]

Modelling studies of supercritical fluid extraction of oils from grape and chia seeds

R. M. Filipe[1,2,*], *J. Coelho*[1,3], *D. Villanueva-Bermejo*[4], *T. Fornari*[4] , *R. Stateva*[5]
[1] *Instituto Superior de Engenharia de Lisboa, IPL, 1959-007 Lisbon, Portugal;* [2] *Centro de Recursos Naturais e Ambiente (CERENA), IST-UL, 1049-001, Lisbon, Portugal;* [3] *Centro de Química Estrutural, IST-UL, 1049-001 Lisbon, Portugal;* [4] *Instituto de Investigación en Ciencias de la Alimentación CIAL (CSIC-UAM). 28049 Madrid, España;* [5] *Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, Bulgaria;*
**rfilipe@isel.ipl.pt*



This work reports the modelling of the kinetics of supercritical extraction of oils from grape seed samples (obtained from a Portuguese industry), and from two sets of chia seeds - high oil content seeds (HOCS), and underutilized low oil content seeds (LOCS). A rigorous thermodynamic framework was applied to calculate the solubility in the supercritical solvent of the grape and chia seeds oils. The oils, for the purposes of modeling, were represented by triolein. Second order polynomial functions are then fitted to the solubility data and used in the kinetics model of Sovová and Stateva [1] to simulate the extraction curves in gPROMS ModelBuilder [2]. The qualitative and quantitative agreement between the experimental and simulated extraction curves in terms of yields was good (2% <AARD < 9%) taking into consideration the very complex nature of the systems examined.

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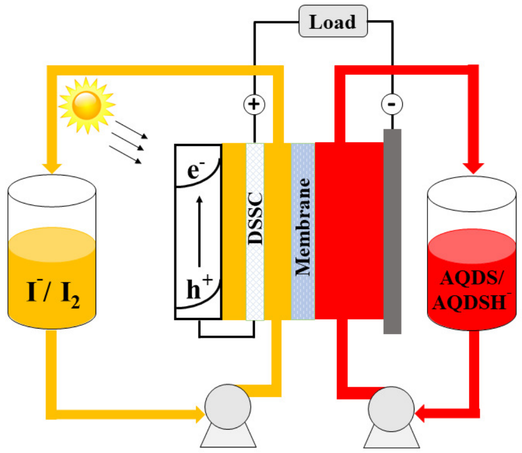
Oral Session

ENERGY AND ENVIRONMENT

[O-EE01]

Unbiased solar charging of an organic-inorganic redox flow battery with a tandem photoelectrode

A. Khataee[1,*], J. Azevedo[2,3], P. Dias[2], E. Dražević[1], A. Bentien[1], A. Mendes[2]
[1]Department of Engineering - Aarhus University, Hangøvej 2, DK-8200 Aarhus, Denmark; [2]LEPABE—Department of Engineering, University of Porto, Rua Dr. Roberto Frias S/N P-4200-465, Porto, Portugal; [3]IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia, Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal.
*khataee@eng.au.dk

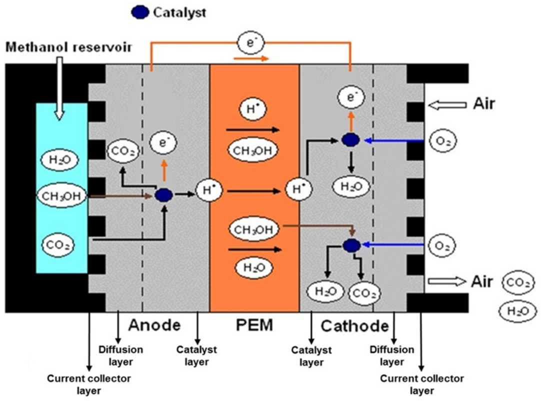


Today, one of the challenges in the renewable energy industry is to store electrical energy in a cost-efficient way. Redox flow batteries have shown great potential, being cost-effective compared to the other technologies. In this work, a solar redox flow cell (SRFC) has been developed to store sunlight directly as chemical energy in liquid electrolyte solutions. An innovative near-neutral organic-inorganic aqueous SRFC is demonstrated using organic and low-cost redox pair anthraquinone-2,7-disulfonate disodium (2,7-AQDS) on the negative side and iodide/iodine (I^-/I_2) redox couple on the positive side. The SRFC yielded a cell potential of ~ 0.8 V. Hematite (α-Fe_2O_3) was used as a photoelectrode and photoelectrochemical characterizations showed a stable performance of α-Fe_2O_3 in contact with iodide/iodine (I^-/I_2) redox couple at pH 5.5, although it is less stable for pH < 7. To charge the SRFC unbiasedly, a tandem system composed of a dye-sensitized solar cell (DSSC) and a α-Fe_2O_3 photoanode was used. The tandem system provided 1.6 V of photovoltage.

[O-EE02]

Optimization of a passive direct methanol fuel cell with different current collector materials

B.A. Braz[1], V.B. Oliveira[1,*], A.M.F.R. Pinto[1,*]
[1] Transport Phenomena Research Center (CEFT), Department of Chemical Engineering, Faculty of Engineering University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal.
* apinto@fe.up.pt; vaniaso@fe.up.pt

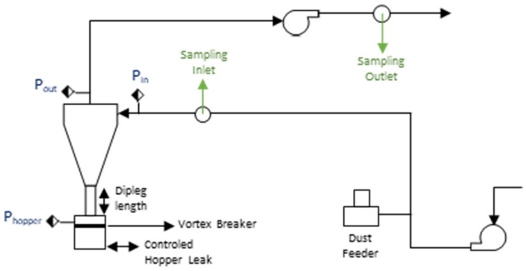


Passive direct methanol fuel cell (DMFCs) are promising devices to replace conventional batteries in portable applications as they use a liquid fuel and offer high energy densities, instant recharging and longer runtimes than batteries. However, to introduce these systems in the market it is mandatory to achieve an optimum balance between its cost, efficiency, reliability and durability. In fuel cells, the current collectors (CCs) ensure the electrons collections, give structural support to the membrane and are responsible for about 80% of the cell total weight. Consequently, to achieve the passive DMFC technology goals (small, compact, low cost and height and high durability and power), CCs should have: high electrical conductivity, corrosion resistance and mechanical strength and low weight and cost. In this work, the effect of the CCs on the DMFC performance is evaluated through the polarization and power density curves and using the electrochemical impedance spectroscopy (EIS).

[O-EE03]

Minimizing non-ideal discharge effects in tangential multicyclone systems

J. Rocha[1], J. Paiva[1,2*], R. Salcedo[1,2]
[1] Advanced Cyclone Systems, SA, R. Vilar, 235, Ed. SCALA, 3Esq, 4050-626, Porto, Portugal; [2] Faculdade de Engenharia, R. Dr. Roberto Frias, s/n, 4200-465 Porto PORTUGAL
* julio.paiva@acsystems.pt

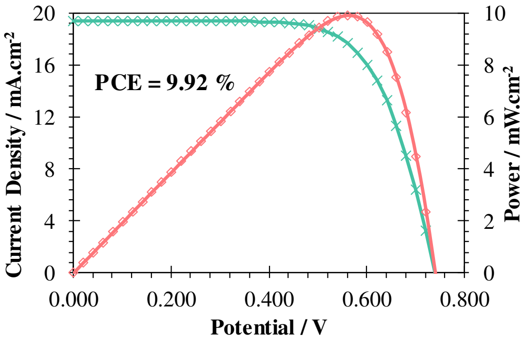


Cyclones are gas/solid separator devices, highly used for the recovery of raw materials and/or to comply with particle emission limits. To design the most compact solution for a multicyclone, a specific optimized geometry was developed, with main focus on scalability, keeping pressure drop and foot-print kept to the minimum possible. This geometry, before being tested on a matrix kind setup (as a typical multicyclone), was tested isolated to evaluate its performance and its sensitivity to non-ideal discharge effects: the dust dipleg length, hopper leakage and the presence of a vortex breaker. The results showed that non-ideal discharge effects may be significant, stressing that air leakages must be avoided. The vortex breaker cannot be neglected, even if the discharge dipleg is kept at an ideal length.

[O-EE04]

Dye sensitized solar cells: guidelines for highly efficient devices based on commercially available materials

C.S. Hora*[1], F. Santos[1], A.I. Pereira[1], J. Maçaira[1], D. Ivanou[1], M.G.F. Sales[2], A. Mendes[1]
[1]LEPABE, Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal; [2]BioMark-CEB/Centro de Engenharia Biológica, Instituto de Engenharia Superior do Porto, Rua António Bernardino de Almeida, 431, 4249-015 Porto, Portugal.
* up200806089@fe.up.pt



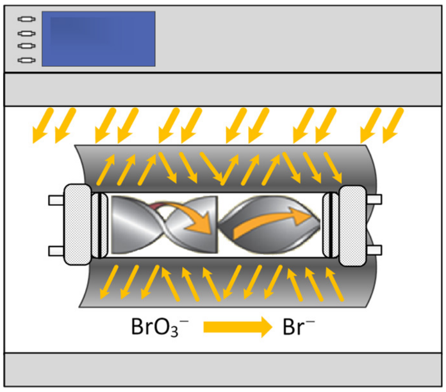
I-V characteristic curve and power curve of the champion DSSC

Commercially available materials were used in the optimization of a high energy efficiency dye-sensitized solar cell (DSSC). The type and thickness of titanium dioxide pastes were optimized to 13 µm of mesoporous paste and 7 µm of scattering paste, post-treated with $TiCl_4$; the combined effect of using a scattering layer and $TiCl_4$ post-treatment made J_{SC} and V_{OC} to increase by 55 % and 6.6 %, respectively. Dipping time, for an efficient sensitization, and DSSC configuration assembly were also optimized; adding chenodeoxycholic acid (CDCA) to the dye and a blocking layer to the photoanode decreased the charge recombination. The final PCE improved from 2.55 % to 9.84 %, under AM 1.5 G one sun light intensity (1000 W·m^{-2}). The best performing DSSC was also characterized under artificial light displaying a PCE of 28.7 % at a light intensity of 1580 µW·cm^{-2} and a PCE of 23.3 % when the light intensity was 225 µW·cm^{-2}. These results are amongst the best performances ever reported.

[O-EE05]

Intensifying heterogeneous TiO_2 photocatalysis for bromate reduction: A static mixer as catalyst support

D. Morais*, F.Moreira, R. Boaventura, V. Vilar
Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.
** daniela.morais@fe.up.pt*

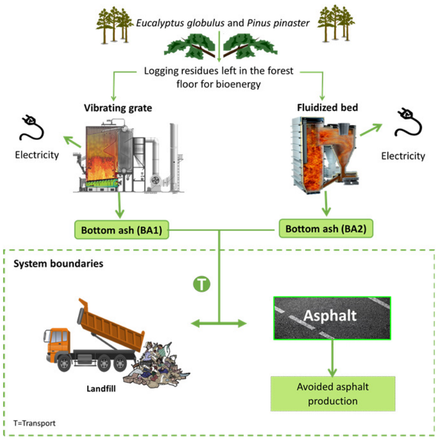


This study focuses on the application of TiO_2 photocatalysis for the reduction of bromate (BrO_3^-) in aqueous solutions using a stainless steel Kenics® static mixer (SM) as support for TiO_2. The SM was assembled in a tubular photoreactor coupled to a compound parabolic collector (CPC) under simulated sunlight. The reuse of TiO_2 films and the effect of the following parameters on the BrO_3^- reduction were assessed: (i) SM pre-treatment, (ii) number of TiO_2 layers deposited on the SM by dip coating, (iii) SM position during coating, (iv) solution pH, (v) solution temperature, (vi) dissolved oxygen (DO) content, and (vii) addition of formic acid (HCOOH) as organic sacrificial agent. TiO_2 films showed a high stability during consecutive reactions. BrO_3^- reduction was favorable under the following conditions: 6 TiO_2 layers, vertical position of the SM during coating, acidic pH and 25 °C. DO had a negative effect on BrO_3^- reduction for pH higher than 5.5. HCOOH had null or negative effect.

[O-EE06]

Life cycle assessment of woody biomass bottom ash valorization in bituminous asphalt

T. P. da Costa*, P. Quinteiro, L. Tarelho, L. Arroja, A. C. Dias
Centre for Environmental and Marine Studies (CESAM), Department of Environment and Planning, University of Aveiro, Aveiro, Portugal.
**tamiris@ua.pt*

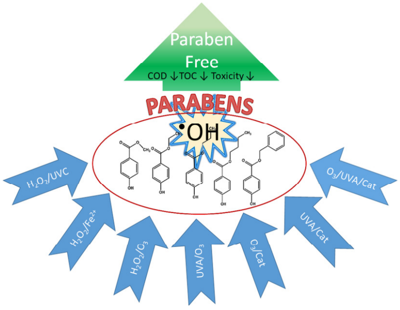


Electricity production from forest biomass to help mitigate climate change is an approach that needs to be planned in order to achieve environmental sustainability. An annual production of 200 thousand tons of woody biomass ash is estimated in Portugal, making waste management an essential issue. The valorisation of woody biomass ash in construction materials appears to be a good management alternative. The purpose of this work is to evaluate the trade-offs between the environmental impacts and benefits associated with bottom ashes incorporation in asphalt production from two different technologies: grate furnace and fluidised bed. Besides, the ash landfill was also evaluated as a base scenario. The results showed that the production of asphalt have a better environmental performance than ash disposal at landfills and appears to be a good alternative for both type of ashes, but the environmental gain is higher using bottom ash from a fluidised bed replacing filler in 10 %.

[O-EE07]

Comparison of radical driven technologies applied for parabens mixture degradation

M. Gmurek[1,2*], *J. F. Gomes*[1], *R. C. Martins*[1], *R. M. Quinta-Ferreira*[1]
[1]*CIEPQPF—Chemical Engineering Processes and Forest Products Research Center, Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, Coimbra, Portugal;* [2]*Faculty of Process and Environmental Engineering, Department of Bioprocess Engineering, Lodz University of Technology, Lodz, Poland.*
[* marta.gmurek@p.lodz.pl](mailto:marta.gmurek@p.lodz.pl)



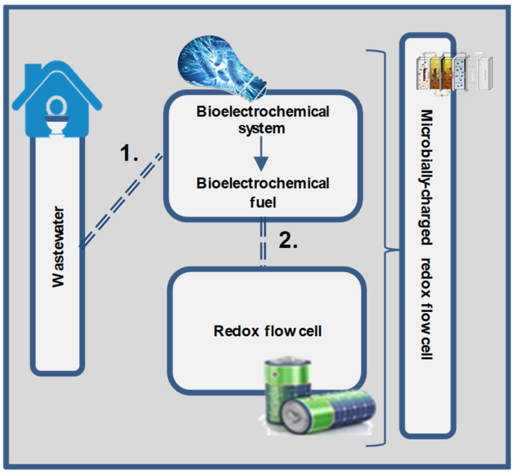
Parabens (esters of p-hydroxybenzoic acid) are a group of commonly used ingredients acting as a preservative in cosmetics and personal care products. They are suspected to be endocrine disruptors. The toxicity of benzylparaben is comparable to bisphenol A. Therefore, it is important to find not only effective but also ecofriendly methods for their removal from aqueous environment.

Herein, the comparison of several radical driven technologies for parabens mixture degradation is presented. H_2O_2/Fe^{2+}, H_2O_2/UVC, O_3/H_2O_2, O_3/UVA, UVA/Cat, O_3/Cat, O_3/UVA/Cat were selected from Advanced Oxidation Processes to degrade parabens from aqueous environment as well as to decrease its toxicity.

[O-EE08]

Bioenergy from wastewater in a microbially-charged redox flow cell

M.S.S. Santos[1,2,3*], *L. Peixoto*[2], *J. Azevedo*[1,4,] *R.A.R. Monteiro*[1,] *C. Dias-Ferreira*[3,5,] *A. Mendes*[1], *M.M. Alves*[2]
[1]*LEPABE, Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering of the University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;* [2]*CEB, Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal;* [3]*CERNAS, Research Centre for Natural Resources, Environment and Society, Coimbra College of Agriculture, Bencanta, 3040-316 Coimbra, Portugal;* [4]*FIMUP and IN–Institute of Nanoscience and Nanotechnology, Department of Physics and Astronomy, Faculty of Sciences of the University of Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal;* [5]*CICECO, Materials and Ceramic Engineering Department, University of Aveiro, 3810-193 Aveiro, Portugal.*
[* marciasofiasantos@hotmail.com](mailto:marciasofiasantos@hotmail.com)



Wastewater is a valuable renewable energy source to generate newest approaches for electrochemical energy conversion in bioelectrochemical system (BES) for energy storage devices. A BES to generate a bio-charging redox pair to be use as negalyte in a redox flow cell (RFC) was study. In BES 2,6-antraquinone was introduced as new redox pair (catholyte), where wastewater mixed communities were the anolyte for the generation of a bio-charged redox pair. The BES results indicated the reduction of the quinone (*ca.* 50 %), promoting power density *ca.* 10 mW m^{-2}. A RFC with the bio-charged redox pair as negalyte and potassium hexacyanoferrate (III) as posilyte was tested, reaching *ca.* 100 % of coulombic efficiency, with potential and energy efficiencies *ca.* 60 %. Wastewater in the new microbially-charged redox flow cell generate a clean energy that can be stored in a new landmark system.

[O-EE09]

Photo-electro-Fenton process for the treatment of highly polluted effluents. Importance of the operational variables

A.M Díez[1,*], *M. Pazos*[1], *M. A. Sanromán*[1]
[1] *Bioengineering and sustainable research group, University of Vigo, Spain;*
**adiez@uvigo.es*

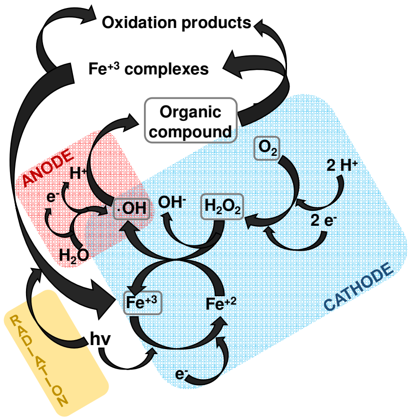
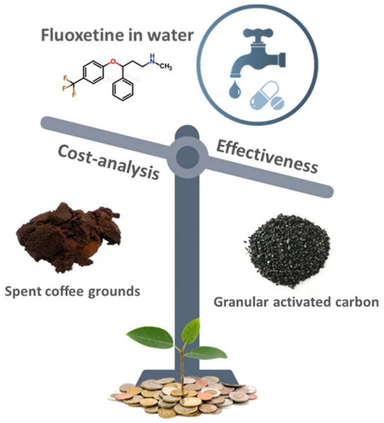


Photo-electro-Fenton processes are a good alternative treatment for the remediation of winery wastewater effluents. The performance of this process can be favored separating the electro-Fenton process from the photo-radiation and thus a two compartment reactor was set. This reactor allowed the adjustment of the distance between electrodes, the modification of the applied voltage, the change of the radiation source and the comparison between different cathodes. All of the above was accomplish in order to enhance the discoloration and mineralization of simulated winery wastewaters. Thus, under the optimal conditions (2 cm of distance between electrodes, 10 V and a prepared highly active cathode), not only the H_2O_2 generation was enhanced but also the remediation of the winery effluent. The results were validated with the treatment of two real wastewater, originating from the white and red wine production industries, and in both cases the results were very encouraging.

[O-EE10]

Valorization of spent coffee grounds as biosorbent for the retention of fluoxetine from water – a cost-effective alternative to activated carbon

B. Silva[1,*], *V. Rocha*[1], *A. Lago*[1], *T. Tavares*[1]
[1] *Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710-057, Braga, Portugal*
** bsilva@deb.uminho.pt*



The goal of this study is to evaluate and to compare the effectiveness of spent coffee grounds (SCG), a waste-based biosorbent, and granular activated carbon (GAC) for the removal of fluoxetine, a widely consumed psychiatric pharmaceutical. Equilibrium measurements performed in batch experiments allowed to determine the adsorption capacity of the materials under evaluation. GAC had by far the highest adsorption capacity, 215.0 mg/g, while SCG showed a maximum uptake of 14.31 mg/g. The cost analysis performed revealed that SCG, although presenting lower adsorption capacity, is the most economically feasible adsorbent, with a cost of 0.77 € per gram of fluoxetine removed, that is quite lower when compared to that of GAC, 1.16 €/g. This study demonstrates that SCG is a waste-based biosorbent that may be successfully applied and be cost-effective for the removal of fluoxetine from water.

[O-EE11]

Carbon dioxide conversion into renewable synthetic fuels, through an electrochemical process

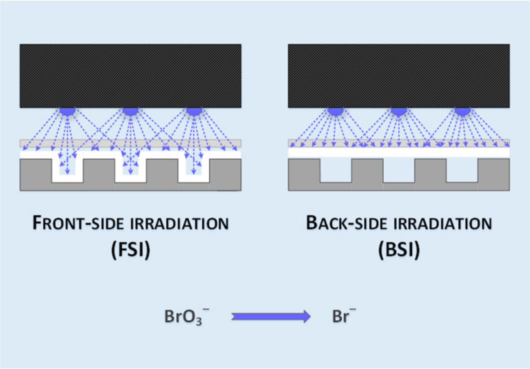
L. Guerra[1,*], *J. Puna*[1,2], *J. Rodrigues*[3], *J. Gomes*[1,2], *M.T. Santos*[1]
[1] Instituto Superior de Engenharia de Lisboa, Rua Conselheiro Emídio Navarro, 1, 1959-007, Lisbon, Portugal; [2] CERENA, IST – Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais, 1049-001 Lisbon, Portugal; [3] GSyF – Green Synthetic Fuel, Clean Energies, Polígono Industrial do Alto do Ameal, Pavilhão C-13, 2565-641 Torres Vedras, Portugal.
** lguerra@live.com.pt*

The environmental sustainability can be supported by the RENEFUEL project, aiming to produce synthetic fuels, such as methane, methanol and di-methyl ether (DME), which can be a renewable alternative to fossil fuels and coal as solutions for mobility. The work, currently under development, is directed to the production of methane from electrochemical technologies, namely through a specific water electrolysis process. The tests carried out, until now, have shown the high potential of this electrochemical process to produce renewable synthetic fuels, an alternative to fossil fuels, with several possible applications, such as rural electrification, in remote locations (for example, islands and mountain villages) and, as an alternative for energy storage or as fuel for mobility.

[O-EE12]

Intensifying heterogeneous photocatalysis for bromates reduction using the NETmix Photoreactor

S. Santos[*], *L. Paulista, T. Silva, R. Boaventura, M.M. Dias, J.C.B. Lopes, V. Vilar*
Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;
** s.santos@fe.up.pt*

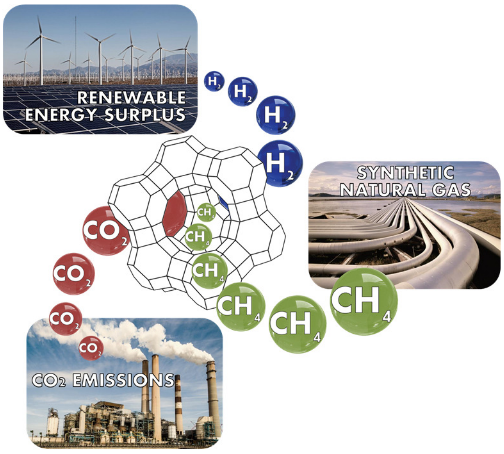


The main goal of this study was the intensification of the heterogeneous TiO_2 photocatalytic process for bromate reduction, using a mili-photoreactor, based on the NETmix technology, irradiated by UVA-LEDs. The BrO_3^- reduction rate was assessed as a function of: i) illumination mechanism, front-side (FSI) vs. back-side (BSI) irradiation; ii) catalyst film thickness; iii) solution pH; iv) solution temperature; and v) absence/presence of oxygen. Higher reduction rates were obtained using the FSI mechanism, mainly associated with a 3-fold increase of catalyst surface area per reactor volume, when compared to BSI. Temperature (15-30ºC) had a negligible effect on the reduction rate. Under the best conditions (stainless steel slab as catalyst support, pH=5.5, 15 mL of a 2% wt. TiO_2 suspension, 25ºC), the reduction rate remained similar for consecutive reactions and almost complete reduction of 200 μg BrO_3^- L^{-1} was achieved after 90 minutes, resulting in $[BrO_3^-] < 10$ μg L^{-1} (guideline value).

[O-EE13]

Zeolite-based catalysts for power-to-gas application: A systematic step by step study for achieving a highly active catalyst

M.C. Bacariza[1,*], I. Graça[2], J.M. Lopes[1], C. Henriques[1]
[1] Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal; [2] Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK.
* maria.rey@tecnico.ulisboa.pt

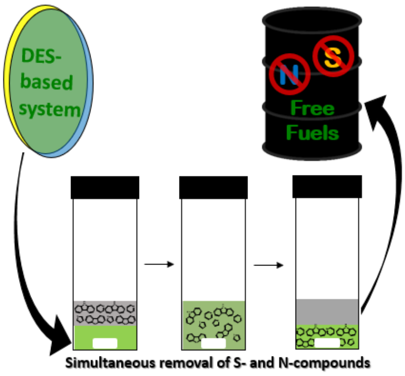


Zeolites could be promising catalysts for power-to-gas due to their tunable properties, potentially interesting for the Sabatier reaction. As CO_2 conversion into CH_4 has been mainly performed over Ni catalysts, in the present work a complete study regarding the optimization of Ni-based zeolites for this reaction was carried out. Thus, the effects of the preparation conditions, the zeolites composition and even the framework type on the catalysts' properties and performances were studied. Then, a promoter of the catalytic activity (Ce) was incorporated to the most promising Ni-Zeolite and the obtained performances in terms of CO_2 conversion and CH_4 selectivity were compared to those of a commercial Ni/γ-Al_2O_3 catalyst. The optimized Ni-Ce/Zeolite from the present work (with CH_4 yield ~80% at 300 ºC) was more active and selective than the commercial catalyst (with CH_4 yield ~30% under the same reaction conditions), proving the suitability of zeolite-based materials for this application.

[O-EE14]

Simultaneous desulfurization and denitrogenation of fossil fuels

F. Lima[1,2,3,4*], A.J.D. Silvestre[2], L.C. Branco[3,4], I.M. Marrucho[1]
[1]Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa; [2]CICECO-Aveiro Institute of Materials and Department of Chemistry, Universidade de Aveiro; [3]Solchemar, Lda; [4]LAQV-REQUIMTE, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa.
* filipa.lima@ist.ulisboa.pt

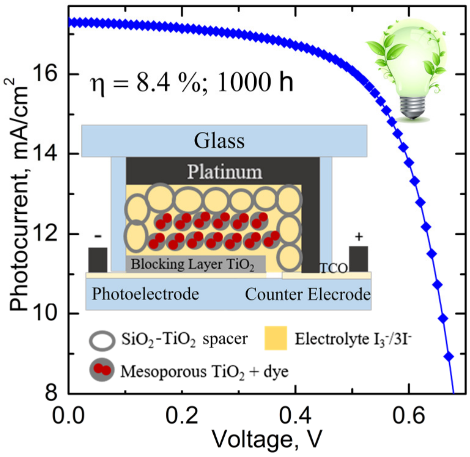


Removal of sulfur and nitrogen compounds from fossil fuels is a key issue, given the stringent legislation and increasing demands for gasoline and diesel quality, as well as the impact on the environment and public health. Hydrotreating process is the current technology used for removal of such compounds in the oil refineries. Nevertheless, it presents several drawbacks, such as, high cost of operation and reduced efficiency in the removal of refractory sulfur compounds. Thus, the search for new and sustainable alternatives or complementary processes is mandatory. Ionic liquids and recently Deep Eutectic Solvents (DES) have been explored as alternative key players for the removal of sulfur and nitrogen from fossil fuels, according several approaches. The aim of this work is focused in the application of new DESs-based systems for the simultaneous extractive desulfurization and denitrogenation of fuels.

[O-EE15]

New ecofriendly cheap spacers for efficient monolithic dye sensitized solar cells

F.E. Santos, D. Ivanou, J. Maçaira, A.I. Pereira, A. Mendes*
LEPABE, Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.
** feosantos92@gmail.com*

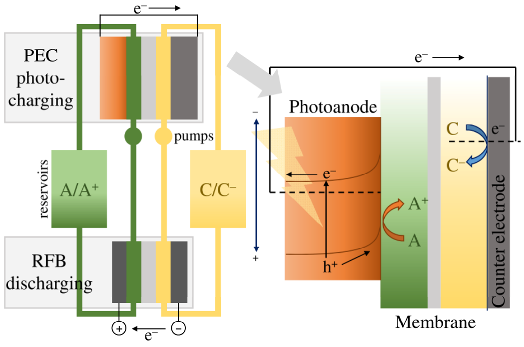


Monolithic configuration is one of the most promising dye sensitized solar cells (DSSCs) architectures; this architecture is easier to fabricate and more compact. Monolithic DSSC were assembled using commercial electrical spacer layers based on ZrO_2 and new cost-effective SiO_2 and SiO_2-TiO_2 insulating layers. For deposition of silica spacers, a water-based formulation (volatile organics free) of silica paste was developed. Porosity and reflectance of the new spacer layers were adjusted to render a monolithic DSSC with high photocurrent conversion efficiency. The best energy performing DSSC comprehends a TiO_2 blocking layer deposited by spray pyrolysis, 20-25 µm TiO_2 photoanode coated with a SiO_2-TiO_2 (70 *wt.* % SiO_2, 30 *wt.* % TiO_2) spacer layer and platinum metal counter electrode of *ca.* 100 nm applied by DC magnetron sputtering. The cell delivered a *PCE* of 8.4 % without aperture mask and 8.3 % with mask – the highest *PCE* ever reported for monolithic DSSCs with liquid electrolyte.

[O-EE16]

Beating the performance of solar charging redox flow batteries based on a hematite photoelectrode

P. Dias[1,], J. Azevedo[1, 2], A. Mendes[1]*
[1]LEPABE - Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal; [2]IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia, Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal;
** pauladias@fe.up.pt*

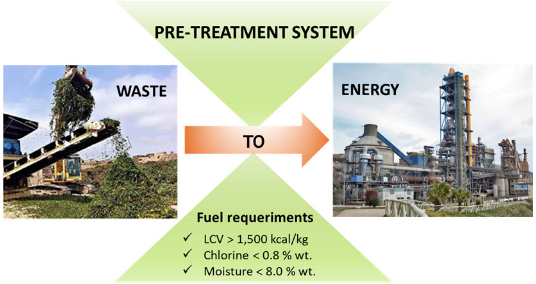


Portugal presents one of the highest solar incidences in Europe, making development of sunlight harvesting and storage technologies very relevant. A solar redox flow cell (SRFC) combines the direct conversion of solar energy into chemical fuels, through the integration of a photoelectrochemical (PEC) cell, for sunlight conversion into both electrochemical and thermal energy, and a redox flow battery for electricity generation. This work reports the optimization of an aqueous alkaline SRFC based on low-cost hematite photoelectrodes and electrolytes consisting of the redox couples ferrocyanide and anthraquinone-2.7-disulphonate in NaOH. Performance improvement strategies are demonstrated for the ferrocyanide-hematite junction, allowing to reach a photocurrent of *ca.* 1.4 mA·cm^{-2} and a photovoltage of 0.8 V. Different hematite surface treatments and cell arrangements were studied and allowed the design of an innovative and very promising SRFC device.

[O-EE17]

Evaluation of different pre-treatment systems for the energy recovery of greenhouse agriculture wastes in a clinker production plant.

L.M.G. Fernández,[1*], *B.N. Rubia*[1], *R.G. Falcón*[2*], *F.V. Borrero*[1]
[1] *School of Engineering of Seville, Department of Chemical and Environmental Engineering, Seville, Spain;* [2] *School of Engineering of Seville, Department of Energy Engineering, Seville, Spain.*
* *lgallego1@us.es*



This study shows the evaluation and selection of the best sequence of operations for the pre-treatment of the wastes derived of the intensive agriculture of greenhouse before recovering their potential energy in the industry. In this research is defined a set of operations aimed at reducing the chlorine percentage and the moisture content present in this kind of wastes for using like an alternative fuel in a clinker production plant. A washing of wastes under optimal conditions could reduce the chlorine content around 60% of the original value and increase the lower calorific value in an 8%. A drying of these wastes with a hot gas stream could produce a recoverable waste with a moisture lower than 3.0 %, which enable the temporary storage avoiding the degradation. The partial substitution of the traditional fossil fuel employed in the clinker production plant involves the reduction of emissions associated with the decrease of the fossil fuel consumption, improvements of the plant operation and economic saving of up to 2.9 € per tonne of clinker produced.

Oral Session

INNOVATIVE MATERIALS AND APPLICATIONS

[O-IM01]

Development of bio- and eco-composites for the footwear industry

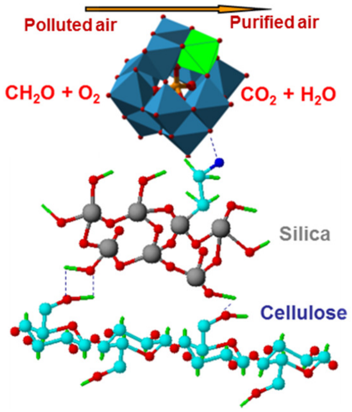
P.C. Santos[1,2,3], I. P. Fernandes[1,2], J. E. Ribeiro[2], J.M.T.A. Pietrobelli[3], M. F. Barreiro[12,]*
[1]LSRE-LCM, Polytechnic Institute of Bragança, Campus Santa Apolonia Ap 1134, 5301-857 Bragança, Portugal; [2]CIMO, Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal; [3]Chemical Engineering Department, Federal University of Technology-Paraná (UTFPR), Campus of Ponta Grossa, 84016-210 Ponta Grossa, PR – Brazil.
[*]barreiro@ipb.pt

Cork composites are often used in several applications including footwear components. The traditional agglomeration process uses a reactive polyurethane-based binder (containing TDI), generating composites with low flexibility and poor water absorption/desorption characteristics, resulting in products with low comfort properties. Furthermore, the presence of TDI, is another important drawback due to its high toxicity. Therefore, the present work is devoted to the development of cork composites, where the TDI-based binder was replaced by an aqueous PUD reinforced with *Melissa officinalis* L. extract. Cork-composites were produced using different adhesive/cork ratios, and characterized in terms of dimensional stability, water absorption/desorption properties, and mechanical behavior. After the selection of the best adhesive content, composites reinforced with sugarcane bagasse, malt bagasse, coconut fibers, and chia seeds were also produced and characterized.

[O-IM02]

Catalytic mineralization of formaldehyde by molybdovanadophosphate polyanions supported on cellulose-silica hybrids

A.R.S. Granja,[1] J.A.F. Gamelas,[2] M.G. Evtyugina,[3] I. Portugal,[1] D.V. Evtuguin[1]*
[1] CICECO, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, P-3810-193, Aveiro, Portugal; [2]Department of Chemical Engineering, CIEPQPF, University of Coimbra, Pólo II—R. Sílvio Lima, 3030-790, Coimbra, Portugal; [3] CESAM, Department of Environment and Planning, University of Aveiro, Campus Universitário de Santiago, P-3810-193, Aveiro, Portugal.
** dmitrye@ua.pt*

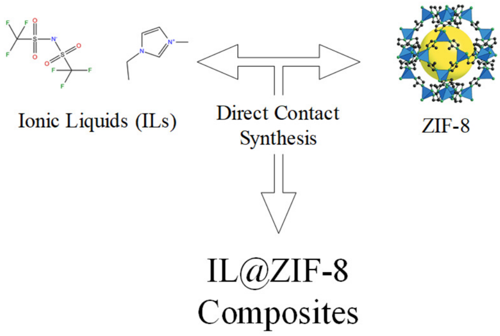


Polyoxometalates (POMs) of series $[PMo_{12-n}V_nO_{40}]^{(3+n)-}$ (n=1,2) supported on cellulose-silica hybrids (*ca.* 2% w/w) exhibited catalytic activity for the gaseous aerobic oxidation of formaldehyde (CH_2O) at room temperature. The oxidation products were carbon dioxide and water. The relative rate of CH_2O oxidation reached values up to 10^{-2} $mol_{CH2O}/(mol_{catalyst}\ s)$, i.e. 4 g/kg of doped hybrid material per sec. The results suggest that catalyst activity is mainly due to active V(V) centres in POMs and that catalyst regeneration by purified air is possible due to reversible turnover V(V)↔V(IV). A mixed electron transfer/autoxidation mechanism was proposed for CH_2O oxidation by the studied catalytic system. According to preliminary estimates, the catalytic system is suitable for sustainable continuous oxidation of CH_2O in polluted air, for concentrations below 50 ppm. This is much higher than the maximum allowable indoor concentration of CH_2O in residential buildings (1-2 ppm).

[O-IM03]

Hybrid ionic liquids/metal organic frameworks – IL@MOFs - for gas separation

T.J. Ferreira[1], A.T. Vera[1], B.Q.C.A. Moura[1], R.P.P.L. Ribeiro[1], J.P.B. Mota[1], L.P.N. Rebelo[1],
J.M.S.S. Esperança[1,], I.A.A.C. Esteves[1,*]*
[1] LAQV - REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, Caparica 2829-516, Portugal
** iaesteves@fct.unl.pt ; jmesp@fct.unl.pt*

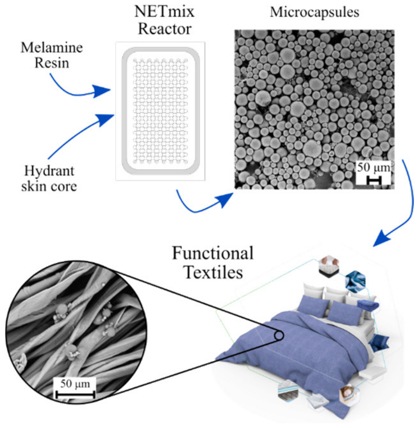


Metal-Organic Frameworks (MOFs) and Ionic Liquids (ILs) stand out as promising alternatives to more traditional materials for gas capture and separation, mainly due to their high gas sorption for CO_2 and their physical and chemical properties. In this work, several combinations of ILs-MOFs, where the IL is impregnated into the MOF structure, were synthesized (IL@MOF) using a direct contact method. Specifically, nine imidazolium-based ILs and a phosphonium-based one were impregnated into ZIF-8. The composites were fully characterized and the CO_2 and CH_4 adsorption-desorption equilibria measurements, in both the pristine ZIF-8 and the IL@ZIF-8 materials, were performed at pressures between 0-16 bar and at a temperature of 303 K. Results confirm the presence of the ILs in the ZIF-8 framework and the stability of the hybrid structures. IL@ZIF-8 materials showed specific surface area and total pore volume losses due to partial IL occupation/blockage of the MOF pores. However, CO_2/CH_4 selectivities of IL@ZIF-8 composites, relative to ZIF-8, show up to a 40% increase in the 0-1 bar pressure range, due to the IL presence. At high pressure, the observed selectivity enhancement is less pronounced.

[O-IM04]

A novel continuous production of melamine based microcapsules with a skin-hydrating active principle for textile applications using the NETmix technology

A.G. Moreira[1], Y.A. Manrique[1], J.C.B. Lopes[1], I.M. Martins[2], A.E. Rodrigues[1], M.M. Dias[1].*
[1]Laboratory of Separation and Reaction Engineering–Laboratory of Catalysis and Materials (LSRE-LCM), Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal; [2]Devan Chemicals, Parque da Ciência e Tecnologia, Rua Eng. Frederico Ulrich, nº2650, 4470-605 Moreira da Maia, Portugal.
** dias@fe.up.pt*

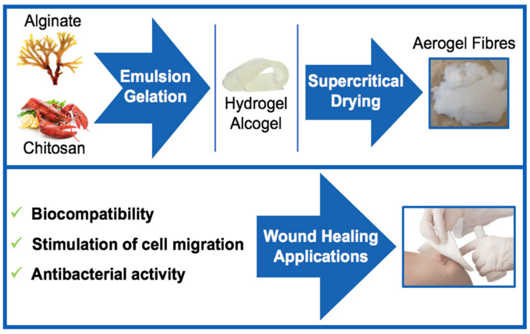


In this work the production of microcapsules for textile applications was developed by adapting the NETmix technology for the steps more commonly made by batch processes: making an oil-in-water emulsion and then curing the membrane around the oily droplets forming microcapsules. Microcapsules were formed through a polycondensation process by coating a skin-hydrating oily active principle with a melamine resin which forms a resistant shell material with a smooth surface. Different temperatures and recirculation times were tested in the cure step. Microcapsules show diameters around 20 µm, within the ideal size range for impregnation on fabrics, and were successfully impregnated on cotton fabrics by a padding process. Integrity and flexible behavior of these microcapsules in the textiles was observed. With the NETmix reactor it is possible to reduce the cure time relative to traditional batch processes, producing microcapsules with similar characteristics in a continuous process.

[O-IM05]

Novel alginate-chitosan aerogel fibres for potential wound healing applications

M. P. Batista[1], *V.S.S. Gonçalves*[1], *F. B. Gaspar*[1], *P. Gurikov*[2], *A. A. Matias*[1]*
[1] *iBET, Instituto de Biologia Experimental e Tecnológica, Apartado 12, 2781-901 Oeiras, Portugal;* [2] *Institute of Thermal Separation Processes, Eißendorferstr. 8, 21073 Hamburg, Germany*
**amatias@ibet.pt*

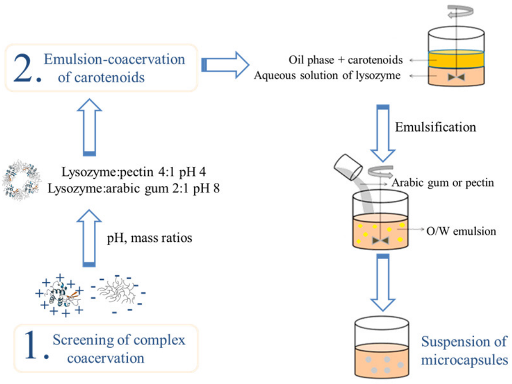


The objective of this study was to produce new alginate-chitosan aerogel fibres and to perform the solid-state characterization, biocompatibility and bioactivity evaluation in order to realize their potential for wound healing applications. The aerogel fibres were prepared by emulsion-gelation method and further dried with supercritical CO_2. The morphology, specific surface area and pore volume as well as the ionic interaction between both polymers and the chitosan content were evaluated. Finally, possible cytotoxicity, *in vitro* cell migration and the antimicrobial activity of these new aerogel fibres were also evaluated. The results of this work demonstrated that the alginate-chitosan aerogel fibres can be considered as having a high potential for wound healing applications.

[O-IM06]

Emulsion-coacervation method for the encapsulation of carotenoids

A. Roda[1], *P. Oliveira*[1], *V.S.S. Gonçalves*[1], *F. Gaspar*[1,2], *A.A. Matias*[1]*
[1] *iBET, Instituto de Biologia Experimental e Tecnológica, Apartado 12, 2781-901 Oeiras, Portugal;* [2] *ITQB, Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de Lisboa, Av. da República 2780-157 Oeiras, Portugal*
** amatias@ibet.pt*



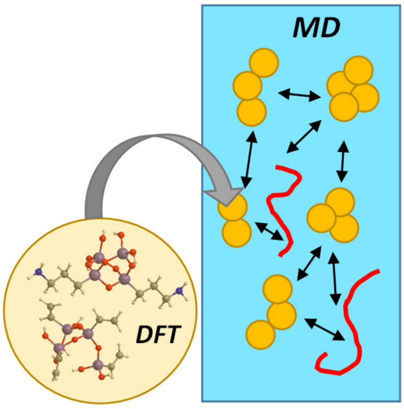
The interest in carotenoids for food and pharma applications as been growing due to its antioxidant activity and its colorant properties. The encapsulation of these compounds to increase its stability and bioavailability has been a target of investigation.

In the present work, an emulsion-coacervation technique for carotenoids encapsulation was studied, using β-carotene as model compound. Coacervation between lysozyme:pectin (L:P) and lysozyme:arabic gum (L:AG) was optimized at different mass ratios and pH values. Coacervates of 4:1 L:P (pH 4) and 2:1 L:AG (pH 8) were selected for encapsulation. Oil-in-water emulsions with lysozyme (aqueous phase) and β-carotene in olive oil (oil phase) were produced and coacerved with the pectin/arabic gum to produce particles. Formation of solid rigid particles was confirmed by scanning electron microscopy and optical microscopy. Load capacities of 0.38 and 1.36 µg β-carotene/mg particle were determined for L:AG and L:P particles, respectively.

[O-IM07]

Insights into polymer-silica aerogel composites from a molecular modelling and simulation approach

M. Oliveira[1], *P. Santos*[1,*], *L. Durães*[1], *P. Simões*[1]
[1] *CIEPQPF, Department of Chemical Engineering, University of Coimbra, 3030-790 Coimbra, Portugal.*
** pmsantos@eq.uc.pt*

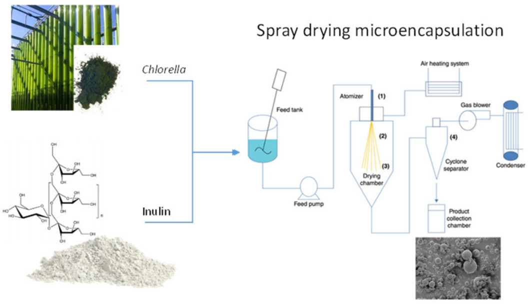


The insertion of polymers into the matrix of silica-based aerogels is an attractive method to improve the mechanical resistance of these materials, and avoid issues hampering their wide-spread use. The engineering of these composite materials ultimately relies on fundamental knowledge about the polymer-silica matrix interactions, but a physical/chemical picture at this level is still largely missing, and hard to achieve with experimental data alone. In this context molecular modelling and simulation techniques have been used in this work to shed light into this subject. A combined experimental and theoretical spectroscopic analysis resulted in a representative microscopic model for the primary particles of the aerogels studied. Subsequent molecular dynamics simulations of composite systems with different polymers revealed the nature of the interactions between the two phases and the effects on the aggregation of silica-based oligomeric species during the composite formation.

[O-IM08]

Microencapsulation of marine *Chlorella* by spray drying

S. Oliveira[1], *M. C. Pereira*[2], *A. Álvarez-Bautista*[3], *N. Fernández*[1], *A. Matias*[1,*]
[1]*Instituto de Biologia Experimental e Tecnológica, Apartado 12, Oeiras, Portugal;* [2]*University of Porto, Rua Dr. Roberto Frias, Porto, Portugal;* [3]*Buggypower Lda., Alameda dos Oceanos, Loja nº 41 Lisboa, Portugal.*
** amatias@ibet.pt*

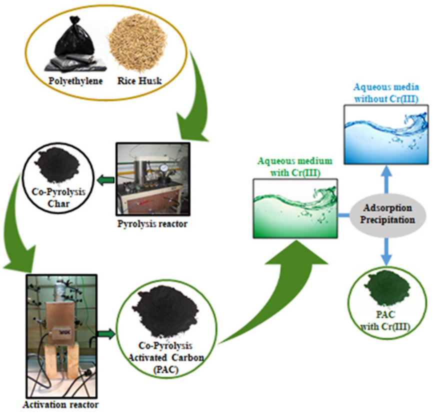


Microalgae technology is a growing field that supports food, feed, pharma and cosmetic industry. Despite their positive effects on health, microalgae products have not gained much importance on food sector, mainly due to their sensorial characteristics (strong color and smell). To overcome this drawback the ability of inulin, a natural prebiotic polysaccharide, as encapsulation matrix is explored. Microparticles of *Chlorella*-inulin were produced by spray drying at different inlet temperatures (120-200 ºC), solid content (5-25%) and wall:core ratios. The optimized microencapsulation process, with a yield of 66%, generated a light powder with a much less intense green tone than the original lyophilized biomass (ΔE=30,35). Microalgae encapsulation led to smaller particles (10 microns) and lower moisture content. In addition, SEM analysis revealed spherical capsules with smooth surfaces, indicative of a good encapsulation efficiency, corroborating inulin's ability to act as a wall agent.

[O-IM09]

Cr(III) removal from aqueous solution by activated carbons obtained through the co-pyrolysis of wastes from rice production

D. Dias[1,*], *M. Bernardo*[2], *N. Lapa*[1], *F. Pinto*[3], *I. Matos*[2], *I. Fonseca*[2]
[1] *LAQV-REQUIMTE, Departamento de Ciências e Tecnologia da Biomassa, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal;* [2] *LAQV-REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal;* [3] *Unidade de Bioenergia, Laboratório Nacional de Energia e Geologia, Estrada do Paço do Lumiar 22, Ed. J, 1649-038 Lisboa, Portugal.*
* *da.dias@campus.fct.unl.pt*

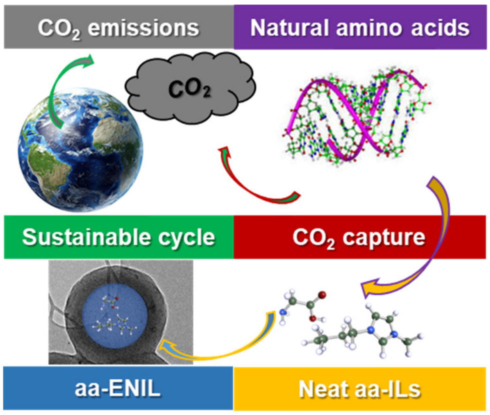


Rice husk and polyethylene were mixed (50 % w/w each) and submitted to pyrolysis. Four physical activation processes with CO_2 were performed on the resulting co-pyrolysis char (PC). The activation at 800 °C, for 4 h, generated the activated carbon (PAC3) with the best textural properties. PC, PAC3 and a commercial activated carbon (CAC) were submitted to Cr(III) removal assays under two S/L: 5 and 10 $g\ L^{-1}$. PC had a high volatile matter content that was removed after the physical activation, resulting in more available pores in PAC3. In Cr(III) removal assays, PC did not remove Cr(III) from the solution, but PAC3 presented similar results to CAC. At the S/L of 5 $g\ L^{-1}$, Cr(III) removal was of 58.5 % for PAC3 and 62.5 % for CAC, both by adsorption mechanism; at the S/L of 10 $g\ L^{-1}$, Cr(III) removal was almost complete due to precipitation caused by pH increase. The highest uptake capacities were of 7.92 $mg\ g^{-1}$ for PAC3 and 8.71 $mg\ g^{-1}$ for CAC, at the S/L of 5 $g\ L^{-1}$.

[O-IM10]

Overcoming the mass transport limitations of amino acid-based ionic liquids in CO_2 chemical absorption by using Encapsulated Ionic Liquids

J. Lemus[*], *R. Santiago, C. Moya, D. Moreno, J. Palomar*[1]
[1]*University Autónoma of Madrid, Chemical Engineering Section. C/ Francisco Tomás y Valiente 7, 28049, Madrid, Spain;*
**jesus.lemus@uam.es.*



The performance of three amino acid-based ionic liquids (aa-ILs) has been evaluated in CO_2 capture by mean of gravimetric measurements. The tested aa-ILs were Bmim with Glycinate, Prolinate and Methionate. First, the CO_2 chemical absorption process was experimentally analyzed by in situ FTIR-ATR, comparing them with theoretical measurements obtained by quantum chemical calculations. This study let us suggest a mechanism of CO_2 chemical absorption on aa-ILs. Then, gravimetric experiments were carried out to characterize the CO_2 capture by aa-ILs. It was found that CO_2 absorption quantification of these ILs was rather slow, because of their high viscosities, so other methodologies had to be employed to quantify the CO_2 capture. In this sense, aa-ILs were encapsulated in porous carbon capsules (aa-ENIL) in order to solve this problem, promoting chemical absorption. The aa-ILs showed considerable higher CO_2 solubility compared to amine cation-based ILs or non-functionalized ILs.

[O-IM11]

Preparation of ceramic and metallic monolithic catalysts for VOC abatement

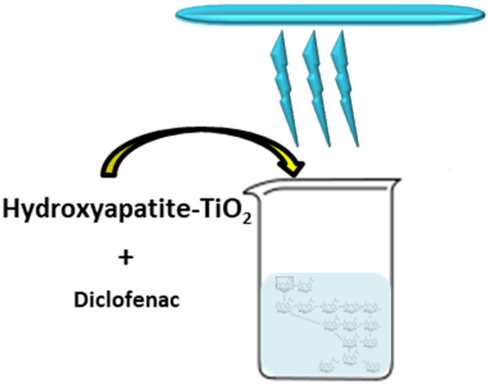
D.F.M. Santos[1,*], *O.S.G.P. Soares*[1], *J.L. Figueiredo*[1], *O. Sanz*[2], *M. Montes*[2], *M.F.R. Pereira*[1]
[1] Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (LSRE-LCM), Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal; [2] Department of Applied Chemistry, University of the Basque Country, Paseo Manuel de Lardizábal 3, 20018, San Sebastián, Spain.
*diogosantos@fe.up.pt.

Cryptomelane-type manganese oxide synthesized by a mechano-chemical method was used as active phase in the preparation of structured catalysts for VOC abatement. Ceramic monoliths with 400 cpsi (cells per square inch) and FeCrAlloy® monoliths with cpsi between 289 and 1330 were used as structured supports. The catalyst slurry was prepared by mixing the active phase in water and adding colloidal alumina to the mixture. The optimization of the slurry was performed by varying the amounts of cryptomelane and colloidal alumina used while monitoring the viscosity of the solution and the amount of mass adhered to a FeCrAlloy® monolith. Several monoliths of the different types were prepared, characterized and tested in the catalytic oxidation of ethyl acetate.

[O-IM12]

Novel hydroxyapatite-TiO_2 composite material for photocatalytic degradation of diclofenac

I.S. Moreira[1*], *S. Murgolo*[2], *C. Piccirillo*[3], *G. Mascolo*[2], *P.M.L. Castro*[1],
[1]*CBQF - Centro de Biotecnologia e Química Fina, Laboratório Associado, Escola Superior de Biotecnologia, Universidade Católica Portuguesa/Porto, Rua Arquiteto Lobão Vital, 172, 4200-374 Porto, Portugal;* [2]*CNR, Istituto di Ricerca Sulle Acque, Via F. De Blasio 5, 70132 Bari, Italy;* [3]*CNR, Institute of Nanotechnology, Campus Ecoteckne, Via Monteroni, 73100 Lecce, Italy.*
* *ismoreira@porto.ucp.pt*

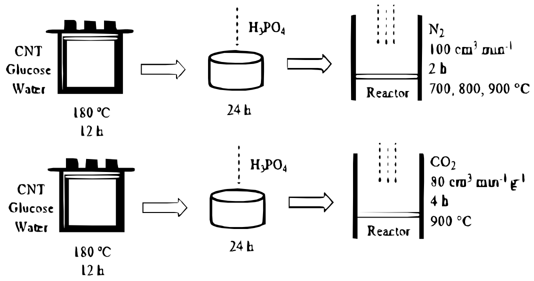


Diclofenac (DCF) is one of the most widely prescribed non-steroidal anti-inflammatory drugs. Since conventional wastewater treatment does not achieve its complete removal, it has been detected in environment. Advanced oxidation processes such as photocatalysis received increasing attention as effective technologies for environmental remediation. In this study, degradation of DCF was investigated by photocatalysis using a new synthetized photocatalyst based on hydroxyapatite obtained from cod fish bones and TiO_2. Degradation of 95% of the target compound was achieved in 24h. Investigation of photo-transformation products was performed by means of UPLC-QTOF/MS/MS their chemical structure was proposed. The toxicity evaluation of final solution was performed using different assays. Overall, the toxicity of the water samples obtained from the photocatalytic experiment decreases, showing the potential applicability of this catalyst for the removal of DCF and detoxification of water matrices.

[O-IM13]

P-doped glucose-derived carbon/carbon nanotubes hybrids for oxygen reduction reaction

R.G. Morais[1], N. Rey-Raap[1], M.A.C. Granja[1], J.L. Figueiredo[1], M.F.R. Pereira[1]*
[1] Associate Laboratory LSRE-LCM, Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, R. Dr. Roberto Frias s/n, 4200-465 Porto, Portugal.
** rgm@fe.up.pt*

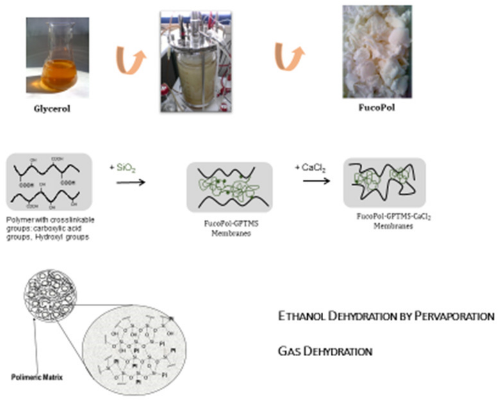


P-doped carbon materials were prepared by the hydrothermal carbonization of glucose in the presence of carbon nanotubes (CNTs), followed by impregnation with phosphoric acid. The materials were used as electrocatalysts in the oxygen reduction reaction (ORR) in order to evaluate the effect of the incorporated functionalities on their catalytic activity. The optimal thermal treatment temperature was found to be 800 ºC, leading to the highest BET surface area and largest incorporation of heteroatoms. Moreover, the combination of chemical and physical activation originated a material with enhanced activity towards the ORR, indicating that impregnation with phosphoric acid improves the electrochemical performance of glucose-derived carbon. electrocatalysts.

[O-IM14]

Hybrid polysaccharide membranes for dehydration processes

I.T. Meireles[1], S.C. Fraga[1], R.M. Huertas[1,2], C. Brazinha[1], C.A.V. Torres[3], M.A. Reis[3], J.G. Crespo[1], I.M. Coelhoso[1*]
[1]LAQV/Requimte, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Campus de Caparica, 2829-516 Caparica, Portugal; [2]Laboratory of Membrane Processes, Instituto de Biologia Experimental e Tecnológica (iBET), apartado 12, 2780-901Oeiras, Portugal; [3]UCIBIO/Requimte, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Campus de Caparica, 2829-516 Caparica, Portugal.
** imrc@fct.unl.pt*



New hybrid polysaccharide (FucoPol) membranes were prepared by incorporation of a SiO_2 network homogeneously dispersed by a sol-gel method with GPTMS as crosslinker.

The hybrid membranes were tested for ethanol dehydration by pervaporation and also for gas dehydration. To mimic industrial dehydration processes, namely flue gas and biogas dehydration, permeation of water vapor, pure gases (CO_2, CH_4 and N_2) and gas mixtures containing 20 vol.% CO_2 + 80 vol.% N_2 and 70 vol.% CH_4 + 30 vol.% CO_2, at different conditions of relative humidity, was monitored by mass spectrometry.

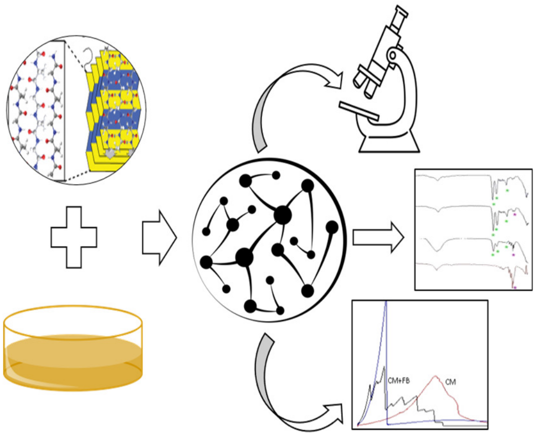
The membranes exhibited high water selectivity values, similar to PERVAP® 4101, however they lost their stability when exposed to solutions of 10.0 wt. % water in ethanol. In contrast, they were stable when applied in gas dehydration with a low gas permeability, while exhibiting high water permeability and selectivity.

[O-IM15]

Production of biomaterial composed by natural polymers

V. S. Soeiro[1], L.L. Tundisi[2], P. G. Mazzola[2], E.B. Tambourgi[3], M. V. Chaud[4], N. Aranha[1], A. F. Jozala[1]*

[1]LaMInFe – Laboratory of Industrial Microbiology and Fermentation Process, University of Sorocaba, Sorocaba/SP, Brazil; [2]Faculty of Pharmaceutical Sciences, State University of Campinas, Campinas/SP, Brazil; [3]School of Chemical Engineering, Campinas State University, Campinas/SP, Brazil; [4]LaBNUS – Laboratory of Biomaterials and Nanotechnology, University of Sorocaba, Sorocaba/SP, Brazil.
**angela.jozala@prof.uniso.br*



Fibroin and bacterial nanocellulose are natural polymers, being used in medicine for bio-dressings and in tissue engineering. Both show great biocompatibility, considering their biodegradability, moldable characteristic and an excellent mechanical and chemical properties, making them a viable option for different applications. For this reason, this study aims a production of films composed of fibroin-bacterial nanocellulose by immersion contact and study their mechanical properties. Fibroin was extracted from *Bombrix mori* and bacterial nanocellulose produced by *Gluconacetobacter xylinus*. The films were produced by immersion contact and characterized by Fourier Transform Infrared Spectroscopy (FTIR spectroscopy) and scanning electron microscopy (SEM). According to the tests, the samples presented excellent properties, which can be explored in other studies, such as tissue engineering.

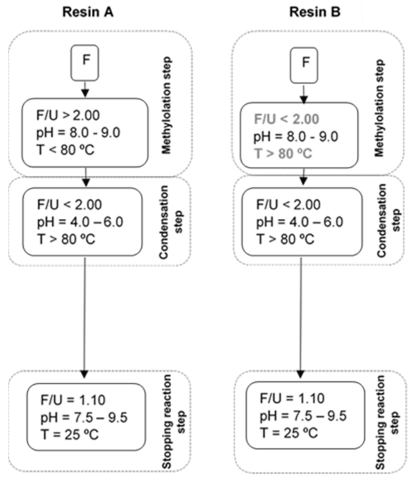
Oral Session

MODELING, SYNTHESIS AND INTEGRATION OF CHEMICAL PROCESSES

[O-MP01]

Influence of synthesis process on urea-formaldehyde resins

C. Gonçalves[1,2], J. Pereira[1,3], N. Paiva[2], J. Ferra[2], J. Martins[1,4], F. Magalhães[1], A. Barros-Timmons[5], L. Carvalho[1,4]*
[1] LEPABE – Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias s/n 4200-465, Porto, Portugal; [2] EuroResinas – Indústrias Químicas SA, 7520-195, Sines, Portugal; [3] ARCP – Associação Rede de Competência em Polímeros, Rua Dr. Júlio de Matos 828/882, Porto, Portugal; [4] DEMad – Wood Engineering Dept., Instituto Politécnico de Viseu, Campus Politécnico de Repeses 3504-510, Viseu, Portugal; [5] CICECO – Aveiro Institute of Materials and Departamento de Química, Universidade de Aveiro, 3810-193, Aveiro, Portugal.
** bio07032@fe.up.pt*

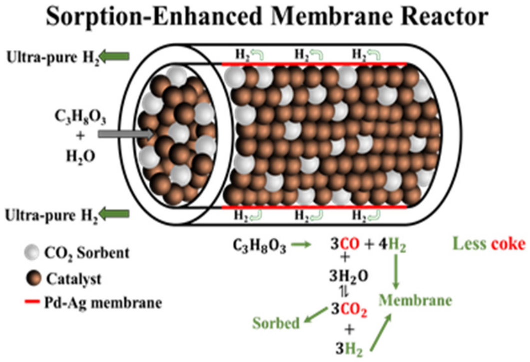


This paper presents the study for two urea-formaldehyde (UF) resins, synthesized using the alkaline-acid process with a final F/U ratio of 1.10 and 1.25. The resins were monitored along the synthesis, trying to better understand the processes involved. The molecular weight distribution of the resins was monitored by Gel Permeation Chromatography/Size Exclusion Chromatography (GPC/SEC) and the unreacted oligomers by High-Performance Liquid Chromatography (HPLC). The samples collected during the reactions under alkaline-acid process were also characterized using quantitative ^{13}C Nuclear Magnetic Resonance (^{13}C-NMR). The GPC/SEC and HPLC data collected during the synthesis showed the growth of the polymer. From these results, and those obtained from ^{13}C-NMR results, it was possible to understand that the differences in chemical structure, for both synthesis are related to methylene linkages and methylol groups. The difference between final F/U ratios (1.10 and 1.25) is also notary for both resins, comparing ^{13}C-NMR. Finally, particleboards (PBs) were produced to evaluate the resins performance.

[O-MP03]

From the traditional packed-bed reactor to the sorption-enhanced membrane reactor: a step towards H_2 production optimization through glycerol steam reforming

*J.M. Silva[1], L.S. Ribeiro[2], J.J. M. Órfão[2], S. Tosti[3], M.A. Soria[1], L.M. Madeira[1],**
[1]LEPABE, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal; [2]Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal; [3]ENEA, Department FSN, C.R. ENEA Frascati, Via E. Fermi 45, Frascati (RM) I-00044, Italy.
** mmadeira@fe.up.pt*

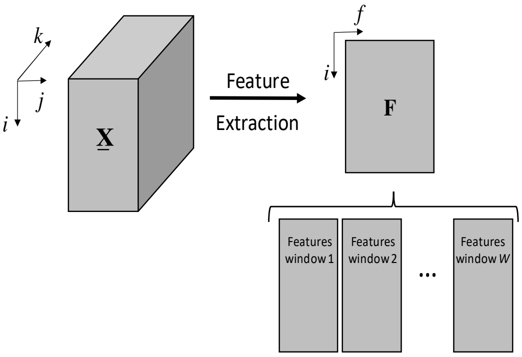


A sorption-enhanced reactor (SER), where a potassium-promoted hydrotalcite was used to capture the CO_2 produced during glycerol steam reforming (GSR) on a Rh-based catalyst, was tested. An enhancement in H_2 production was observed not only during the CO_2 pre- and breakthrough, but also during the post-breakthrough as compared to the traditional reactor – TR. Considerably higher H_2 purity was obtained in the first moments. A much significant improvement in H_2 production was observed in the sorption-enhanced membrane reactor (SEMR), where H_2 was selectively separated by a Pd-Ag membrane. An increment from 1.6, in the SER, up to 3.6 mol of H_2 per mol of fed glycerol was obtained. Besides the ultra-pure H_2 obtained in the permeate side of the Pd-Ag membrane, highly pure H_2 was also obtained in the retentate side before the breakthrough, meaning that if the SEMR is continuously operated in the pre-breakthrough, pure H_2 would continuously be obtained in both retentate and permeate streams.

[O-MP04]

Window-based feature methods for end-of-batch quality prediction

R. Rendall[1], *I. Castillo*[2], *A. Schmidt*[2], *S.T. Chin*[2], *L. Chiang*[2], *M. Reis*[1,*]
[1] *Department of Chemical Engineering, University of Coimbra, Rua Sílvio Lima, Coimbra, Portugal;* [2] *Dow Chemical Company, Freeport, TX, USA;*
* *marco@eq.uc.pt*

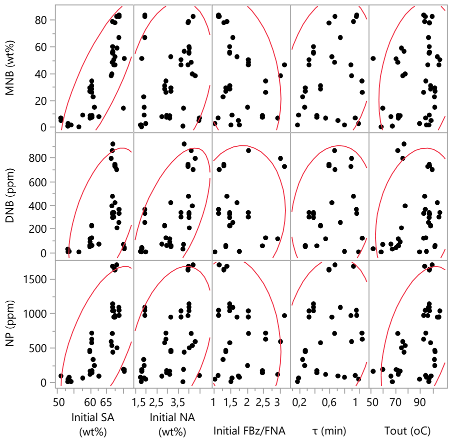


Batch processes are ubiquitous in modern industry and batch data analysis is an important task for improving process operation. In this context, feature-oriented methods are effective methodologies that have the key advantage of not requiring complex data preprocessing, such as synchronization. However, these methods lack time-resolution since features are extracted for the full duration of the batch or batch stage. Thus, in this work, we propose a class of methods based on features with time localization, called window-based features (WiF). The underlying idea consists in extracting features from small windows of data, thus enhancing the time-resolution capabilities of feature-oriented methods. Two simulated case studies are considered to test the proposed approach. In both cases, WiF presents similar or better prediction performance when compared to other benchmarks and also presents an improved ability to easily identify relevant process variables and locate important batch periods.

[O-MP05]

Nitration process intensification

A.L.C.V. Lopes[1,2,3], *D.C.M. Silva*[1], *I. Portugal*[3], *C.M.S.G. Baptista*[2,*]
[1] *Bondalti Chemicals S.A., Quinta da Indústria, R. Amoníaco Português nº10, Beduído, 3860-680 Estarreja, Portugal;* [2] *IEPQPF - Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, R. Sílvio Lima, Polo II, 3030-790 Coimbra, Portugal;* [3] *Department of Chemistry and CICECO, University of Aveiro, Campus Universitário de Santiago, 3810 - 193 Aveiro, Portugal.*
* *cristina@eq.uc.pt*

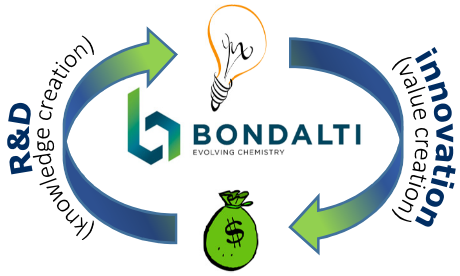


The liquid-liquid nitration of benzene to mononitrobenzene (MNB) still faces restrict environmental regulations related to the formation of by-products such as nitrophenols (NP) and dinitrobenzenes (DNB). Microreactors have proven their potential to conduct hazardous and/or multiphasic reactions limited by mass and heat transfer with high-performance results. Benzene nitration was carried out in a Corning® Low-Flow Reactor (LFR) microreactor to study the influence of the main operating variables on conversion and by-products formation. The most influent were the initial composition of the aqueous phase in sulfuric (SA) and nitric (NA) acids and the reactor outlet temperature (T_{out}). The use of a strongly acidic media, higher operating temperature, an intermediate residence time (τ) and a lower stoichiometric excess of benzene to HNO_3 (F_{Bz}/F_{NA}) promoted high conversion (< 99.9 %). Lower NP and similar or higher DNB concentrations were achieved, being most of them lower than 1000 ppm.

[Bondalti]

R&D+i at Bondalti

P. Araújo[*]
Bondalti CHEMICALS, S.A. Quinta da Indústria, Rua do Amoníaco Português, nº 10 Beduído, 3860-680 Estarreja, Portugal;
[*] paulo.araujo@bondalti.com



The R&D+i creation cycle

CUF, the chemical industry business area of the José de Mello Group, officially announced at the end of May 2018 the change of its corporate identity, a new brand called Bondalti. The new Bondalti brand, which succeeds the historic CUF brand, is the culmination of a strategic repositioning process, which now enters a phase of more growth, more ambition, more innovation and, most of all, more internationalization. Innovation is one of the values of Bondalti and the company is strongly commitment to using science and technology to develop new processes and products. In 2017, roughly 26% of the workforce was engaged in Research, Development and Innovation (R&D+i).

[O-Prio]

PRIO: a perspective for a more sustainable mobility

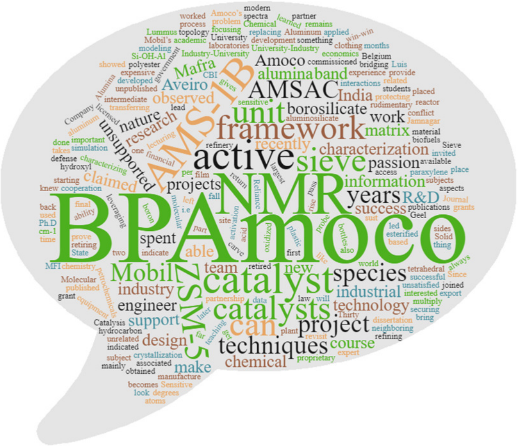
C. Correia[1]
[1] *PRIO, Terminal de Granéis Líquidos, lote D, Porto de Aveiro, 3834-908 Gafanha da Nazaré, Portugal.*
cristina.correia@prioenergy.com

Since 2006 PRIO distributes and commercializes liquid fuels and LPG, having a tank terminal located in Aveiro (for stockage and independent primary logistics) as well as its own biodiesel factory. It is 100 % funded by Portuguese capital and is the only Iberian gas company with the triple certification for quality, safety and environment. PRIO's network includes over 200 fuel stations across Portugal. With a continuous focus on more sustainable options for mobility, PRIO has been sharing its challenges with the scientific community along the years. More recently, PRIO has launched JUMP Start, an open innovation programme especially designed for startups. In PRIO we believe that a more sustainable mobility is possible, and that open innovation is the quickest way to achieve it.

[O-BP]

Solid-State NMR characterization of the BP Amoco AMS-1B borosilicate molecular sieve

J. Amelse,[1,*] P.V. Wiper[1], L. Mafra[1], A. Hough[2], A. F. Routh[2], S. A. Clarke[2]
[1] Department of Chemistry, CICECO – Aveiro Institute of Materials, University of Aveiro, Campus Universitário de Santiago 3810-193, Aveiro, Portugal; [2] Department of Chemistry, Cambridge University, UK.
jamelse@ua.pt



AMS-1B is a borosilicate molecular sieve that has an MFI framework topology like Mobil's ZSM-5 aluminosilicate sieve. Unsupported AMS-1B is not active. It becomes active when placed in an alumina matrix. Mobil claimed that activation takes place by aluminum from the matrix replacing boron in the sieve framework. Aluminum in the framework of ZSM-5 gives rise to a band in IR spectra at 3610 cm^{-1} associated with an Si-OH-Al bridging hydroxyl, which is the active acid site in ZSM-5. As far back as the 1980's we showed that this band is not observed in active AMSAC catalysts. While, IR indicated that the active Al species in AMSAC catalysts is different than that in ZSM-5, it did not indicate what it is. That is a problem that bothered me for 30 years. Thirty years later I received a grant from BP to work with Dr. Luis Mafra at the University of Aveiro to revisit the problem with modern Solid State NMR techniques, which only became available very recently. These include cross polarization techniques that can probe interactions between Al or B and neighboring atoms. I will describe results from our efforts which led to two publications in the Journal of Catalysis.

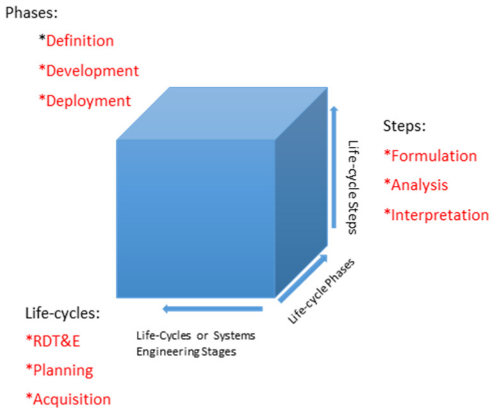
Oral Session

MULTISCALE AND MULTIDISCIPLINARY ENGINEERING EDUCATION

[O-ME01]

Introduction to systems engineering and sustainability for chemical and biological engineers

U. Tuzun[1,*]
[1] Alumnus Professor, University of Cambridge; Cambridge, United Kingdom
* prof.ugur.tuzun@cantab.net

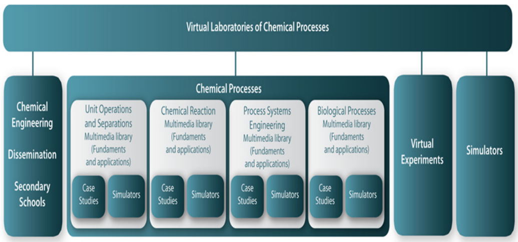


A multi-disciplinary systematic teaching approach is illustrated supplemented by industrial case studies. The multidisciplinary concepts are introduced by first starting with introduction of the academic/professional learners to systems thinking and creative problem solving methodology with illustrations of their application in fundamental engineering design concepts. The teaching then continues to introduce the learner to the fundamentals of sustainable development with specific examples of application drawing together environmental, socio-economic and engineering design principles. The learner is enabled to recognize simple and complex systems, identify sub-systems and with the use of specific examples, is trained to undertake systems integration in engineering process design. Specific examples of the applications of integration management include the interactions between process systems, environmental and bio-systems and socio-economic enterprise systems in sustainable development; see for example, Smith [1].

[O-ME03]

Virtual labs: Tools to enhance students autonomy in Chemical Engineering education

M.G. Rasteiro[1,*], D. Urbano[2], J. Granjo[1]
[1] CIEPQPF, Department of Chemical Engineering, University of Coimbra, Rua Sílvio Lima – Pólo II, Coimbra, Portugal;
[2] University of Porto, FEUP, Porto, Portugal.
* contact_mgr@eq.uc.pt



Engineering educators have been driven to develop different approaches to supplement scientific background and further develop the capacity for autonomous and critical thinking in students. In 2009, the University of Coimbra has made available on-line a virtual platform with a wide scope, directed towards Chemical Engineering education. The platform is divided into four different educational topics: Unit Operations and Separations, Chemical Reaction, Process Systems Engineering and Biological Processes. These sections include simulators, applications and case studies to help understanding chemical/biochemical processes. The ultimate objective was to help students in their autonomous study and, thereafter, in developing their capacity of autonomy. This paper presents an assessment of the use of that platform by two different groups of students: a group from the 3rd year of the 1st cycle of Chemical Engineering, and another one from a Project Design course (2nd cycle, MSc of Chemical Engineering).

[O-ME04]

Understanding the effect of oxygen on microbial growth – teaching bioprocess engineering to biotechnology students

A.M.R.B. Xavier[1], *L. S. Serafim*[1]
[1] *CICECO – Aveiro Institute of Materials, Departamento de Química, Universidade de Aveiro, Aveiro, Portugal.*
luisa.serafim@ua.pt

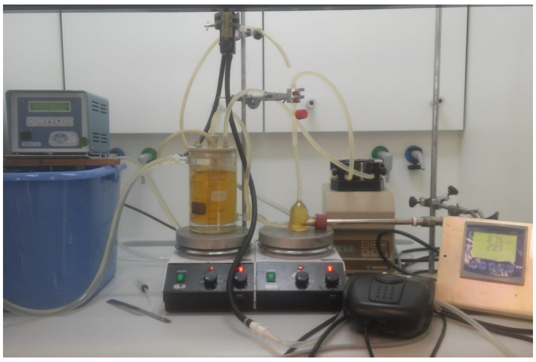


Figure 1 – Experimental setup

The study of metabolic behavior of cell cultures along with the operation of bioreactors is of extremely importance for students of Biotechnology and Chemical Engineering. The objective of this laboratorial work was to consolidate the theoretical concepts acquired by students, and understand how bacterial growth, nutrients consumption and oxygen uptake can be correlated in biological systems. A batch bioreactor with controlled temperature, agitation and aeration was used to grow a culture of *Saccharomyces cerevisiae*. The measurement of oxygen concentration was carried out in a reactor connected to a respirometer in which was introduced an oxygen sensor. This work required around 8 h and ran continuously throughout a day. Students divided their tasks and shared their experimental results with colleagues for further analysis and data processing to determine kinetic and stoichiometric parameters. The balance of in this practical work was very positive, since students apprehended the link between the metabolic functions and process variables, as well as they learnt methods of calculation and organization of information, in addition to acquisition of team work skills.

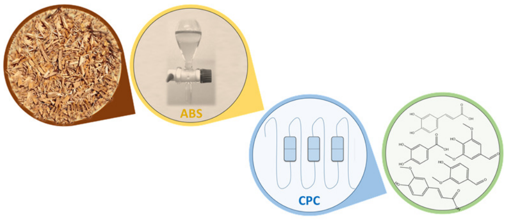
Poster Session

BIOLOGICAL ENGINEERING AND BIOTECHNOLOGY

[P-BB01]

Centrifugal partition chromatography on the separation of phenolic compounds derived from lignin depolymerization

J.H.P.M. Santos[1]*, M.R. Almeida*[1]*, A.C.R.V. Dias*[2]*, M.G. Freire*[1]*, J.A.P. Coutinho*[1]*, S.P.M. Ventura*[1]***
[1] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;* [2] *CESAM – Centre for Environmental and Marine Studies, Department of Environment and Planning, University of Aveiro, 3810-193 Aveiro, Portugal.*
**spventura@ua.pt*

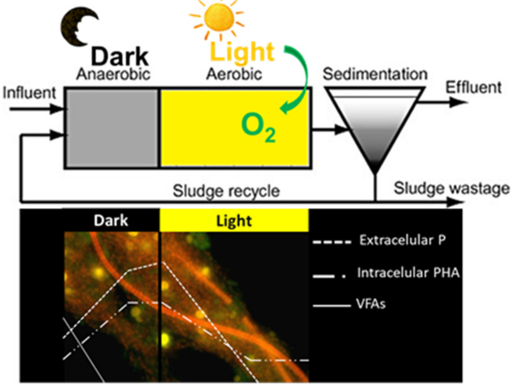


Phenolic compounds are ubiquitous biomolecules exhibiting a wide range of physiological properties, with application in the pharmaceutical and nutraceutical fields. Here, aqueous biphasic systems (ABS) formed by polyethylene glycol, sodium polyacrylate, and inorganic salts or ionic liquids as electrolytes, were applied to purify caffeic, ferulic and protocatechuic acids, vanillin and syringaldehyde. After the proper optimization, the best system was applied in centrifugal partition chromatography (CPC) allowing the efficient compounds separation, while demonstrating the potential of polymer-based ABS to be used in CPC. The recovery of the phenolic compounds (between 65 and 87%) with high purity from the ABS phases was carried, allowing to reuse the ABS phases, which was proved to be of low environmental impact. Actually, in a scenario where the polymeric phases are reused, the carbon footprint is decreased to 36%, as the consumption of new chemicals and water reduces considerably.

[P-BB02]

Phototrophic enhanced biological phosphorus removal: A solution for reducing the aeration necessities in conventional enhanced biological phosphorus removal systems

V. Carvalho[1*]*, E. Freitas*[1]*, P. Silva*[1]*, J. Fradinho*[1]*, A. Oehmen*[1]*, M. Reis*[1]
[1] UCIBIO-REQUIMTE, Department of Chemistry Faculty of Sciences and Technology, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal; [2] School of Chemical Engineering, University of Queensland, Brisbane, QLD, 4072, Australia.
* virginiacfcarvalho@gmail.com

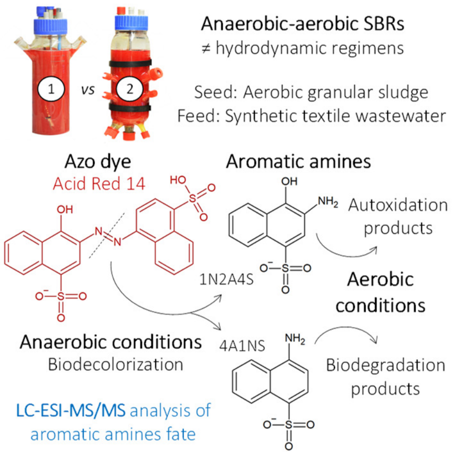


An innovative Phototrophic - Enhanced Biological Phosphorus Removal (Photo-EBPR) system, consisting of a consortium of photosynthetic organisms and polyphosphate accumulating organisms (PAOs), was studied in this work. A sequencing batch reactor fed with a mixture of acetate and propionate was subjected to dark/light cycles in order to select a photo-EBPR system containing PAOs and photosynthetic organisms, the system oxygen providers. The results showed that the photo-EBPR culture can perform P release in the dark and has high capacity of P removal in the light phase in the absence of air or another electron acceptor. These results indicated that a photo-EBPR system can be a potential solution for P removal with low COD/P ratios and in the absence of aeration, prospecting the use of natural sunlight as illumination, which would reduce the costs of EBPR operation regarding aeration.

[P-BB03]

Biodegradation of a sulfonated azo dye in anaerobic-aerobic bioreactors treating a simulated textile wastewater investigated by liquid chromatography-tandem mass spectrometry

R.D.G. Franca[1], M. Conceição Oliveira[2], H.M. Pinheiro[1], N.D. Lourenço[1,3,]*
[1] iBB – Institute for Bioengineering and Biosciences, Department of Bioengineering, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal; [2] Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal; [3] UCIBIO, REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Campus de Caparica, 2829-516 Caparica, Portugal.
** nidia.lourenco@fct.unl.pt*

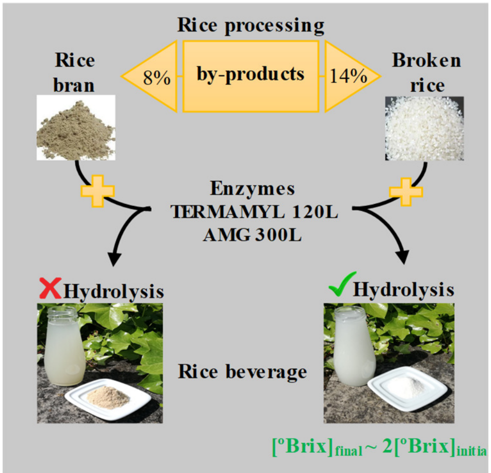


This study compared two anaerobic-aerobic sequencing batch reactors (SBRs) operated under different hydrodynamic regimens, regarding the treatment performance of a synthetic textile wastewater, with a focus on azo dye (Acid Red 14, AR14) biodegradation. Liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) was used for structural characterization of AR14 biodegradation metabolites, their molecular formulae being confirmed by high resolution MS/MS. The SBRs shared most of the identified compounds (32 molecules), but differences were observed in their metabolite aerobic profiles. Biodecolorization via AR14 anaerobic reduction was confirmed by the identification of the sulfonated aromatic amine 4A1NS, which was further aerobically biodegraded, involving aromatic ring deamination and hydroxylation. The other aromatic amine (1N2A4S) was not detected, probably undergoing autoxidation reactions. A new AR14 biodegradation pathway was observed upon supplementation with nitrate.

[P-BB04]

Technological aspects of beverage production using rice processing by-products: Bran and broken rice

D. Silva[1], A. Borges[1,], M. Henriques[1,2], I. Rodrigues[1,2]*
[1] Polytechnic Institute of Coimbra, College of Agriculture, Bencanta, PT-3045-601 Coimbra, Portugal; [2] Research Centre for Natural Resources, Environment and Society (CERNAS), College of Agriculture, Polytechnic Institute of Coimbra, Bencanta, PT-3045-601 Coimbra, Portugal.
**raquel.borges@esac.pt*



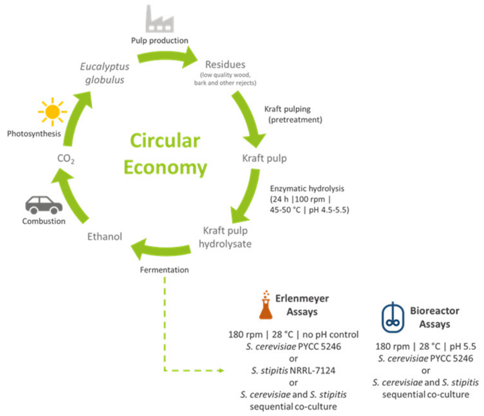
Agroindustry activities generate different types and quantities of by-products. Their valorization is a challenge for industries and has a great importance in circular economy. Rice processing by-products have a great potential for valorization.

This work intended to study and optimize the enzymatic hydrolysis of two rice by-products (bran and broken rice) for the development of rice-based beverages. Two commercial enzymes were used for starch hydrolysis alone or in combination. For broken rice, using TERMAMYL 120L the reducing sugars profile was similar to the one found where both enzymes were applied. In the case of rice bran, due to its small amount of starch, it was observed an absence of enzymes activity. Under the tested conditions, broken rice proved to be a viable solution for the development of rice-based beverages without sugars addition, in contrast with rice bran. Besides that, the exclusive application of TERMAMYL 120L simplifies the production process and reduces costs.

[P-BB05]

Biethanol production from Kraft pulp in a circular economy perspective

R.H.R. Branco[1,*], J.G. Pinho[1], L.S. Serafim[1], A.M.R.B. Xavier[1]
[1] CICECO – Aveiro Institute of Materials, Departamento de Química, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal.
*rebola@ua.pt

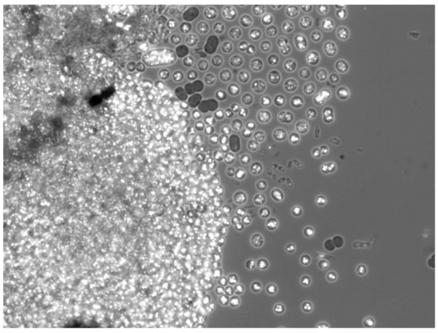


Bioethanol is a potential alternative to fossil fuels, which have negative impact in health and environment. Bioethanol is mainly produced from food crops, leading to food-fuel competition. Second generation bioethanol is produced from lignocellulosic biomass (LCB), requiring a costly and technically difficult pretreatment. Kraft pulping removes lignin, releasing cellulose, and can be considered as a pretreatment. Kraft pulping followed by hydrolysis of polysaccharides and fermentation is a promising approach to valorise wastes resulting from pulp and paper industry and can be integrated in a biorefinery. This work studied the production of bioethanol from unbleached Kraft pulps of *Eucalyptus globulus*. Hydrolysis of the Kraft pulp allowed a hydrolysis yield of 95.6 ± 2.6 %. The sequential co-culture of *Saccharomyces cerevisiae* and *Sheffersomyces stipitis* was the most effective assay, with a maximum ethanol concentration of 20.0 ± 0.6 $g.L^{-1}$, and an ethanol yield of 0.464 ± 0.009 $g.g^{-1}$.

[P-BB06]

Polyhydroxyalkanoates production from agricultural wastes and domestic wastewater with phototrophic purple bacteria

J.C. Fradinho[1, *], B. Pereira[1], J. Almeida[1], A. Oehmen[2], M.A.M. Reis[1]
[1] UCIBIO-REQUIMTE, Department of Chemistry, Faculty of Sciences and Technology, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal; [2] Present address: School of Chemical Engineering, University of Queensland, Brisbane, QLD, 4072, Australia.
* j.fradinho@campus.fct.unl.pt



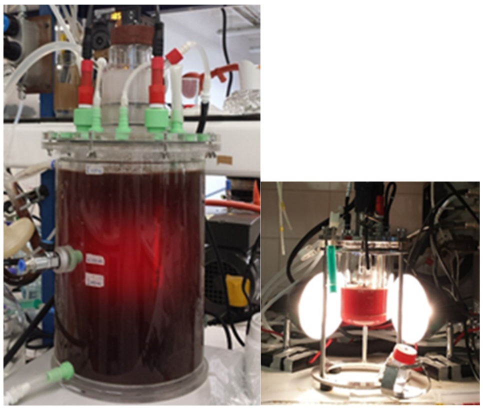
Fluorescence microscopic picture of Nile blue staining showing cocci shaped phototrophic purple bacteria accumulating PHA

Polyhydroxyalkanoates (PHAs) are biodegradable biopolymers with physical-chemical properties similar to conventional plastics. They can be produced by several microorganisms including phototrophic purple bacteria (PPB). Currently, two Horizon 2020 European projects, INCOVER and NoAW are studying operating strategies to valorize agricultural wastes and domestic wastewater via PHA production with mixed cultures of PPB. The strategies developed thus far, led to PHA accumulation values of up to 20% PHA/VSS in the INCOVER selector reactors, and up to 30% in accumulation tests. NoAW attained a PHA content of 15 % PHA/VSS with synthetic feed simulating fermented manure. It is expected that the studies developed under these two projects will provide answers to address the request for a sustainable plastic production system that comprises the utilization of renewable feedstocks and a cost-effective production of biodegradable plastics.

[P-BB07]

Optimization of operating conditions in accumulator reactors for improved polyhydroxyalkanoates production with phototrophic purple bacteria

J. C. Fradinho[1, *], *A. Oehmen*[2], *M.A.M. Reis*[1]
[1]*UCIBIO-REQUIMTE, Department of Chemistry, Faculty of Sciences and Technology, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal;* [2]*Present address: School of Chemical Engineering, University of Queensland, Brisbane, QLD, 4072, Australia.*
**j.fradinho@campus.fct.unl.pt*

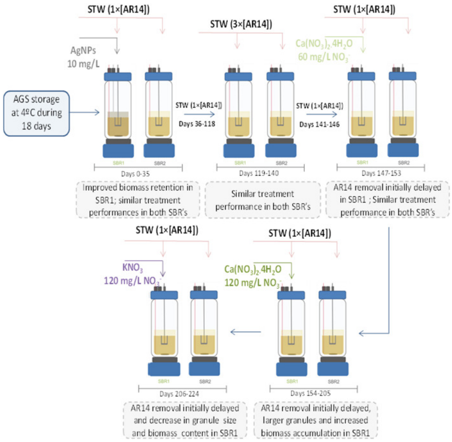

Selector reactor enriched in phototrophic purple bacteria (left) and accumulator reactor (right)

Phototrophic mixed cultures (PMCs) were recently proposed as new microbial systems for polyhydroxyalkanoates (PHAs) production. These cultures can be selected under the permanent presence of carbon and the PHA production can be enhanced in a subsequent accumulation step. To optimize the PHA production in accumulator reactors, this work evaluated the impact of two different operating conditions on the culture performance: initial acetate concentration and light intensity. Results indicate that the highest PHA production rates can be obtained when operating the accumulator reactors at low acetate concentration (< 30 CmM) and specific light intensities around 20 W/g *X*. Also, it was shown for the first time, the capability of a PMC to use a real waste, fermented cheese whey, to produce PHA with an HV content of 12%. These results confirm that cheap VFA-rich fermented wastes can be used as substrates for PHA production with PMCs and prospect the operation under direct sunlight illumination.

[P-BB08]

Impact of textile wastewater composition on the performance and properties of an aerobic granular sludge-sequencing batch reactor system during operation after granule storage

A.M. Rodrigues[1], *R. Rosa*[1], *R.D.G. Franca*[1], *H. Pinheiro*[1], *N.D. Lourenço*[1,2*]
[1] *iBB – Institute for Bioengineering and Biosciences, Department of Bioengineering, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal;* [2] *UCIBIO, REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Campus de Caparica, 2829-516 Caparica, Portugal.*
** nidia.lourenco@fct.unl.pt*

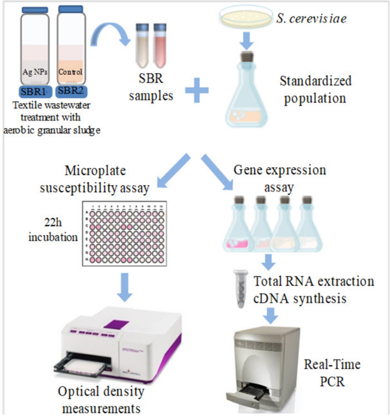


In this study, two sequencing batch reactors (SBR) were inoculated with aerobic granular sludge (AGS) previously used to treat simulated textile wastewater containing the azo dye Acid Red 14 and stored for 18 days at 4ºC. The effect of silver nanoparticles (AgNPs, 10 mg/L) was assessed during AGS reactivation, its supply being interrupted after 35 days of operation. The impact of changes in wastewater composition on AGS properties and treatment performance was studied, including a three-fold increase in the concentration of dye, and the addition of nitrate salts, namely $Ca(NO_3)_2{\cdot}4H_2O$ (60 and 120 mg NO_3^-/L) and KNO_3 (120 mg NO_3^-/L). AgNPs and $Ca(NO_3)_2{\cdot}4H_2O$ seemed to have promoted granulation and biomass accumulation. Color and organic matter removal yields of around 80% were obtained, irrespective of the presence of AgNPs. The addition of $Ca(NO_3)_2{\cdot}4H_2O$ or KNO_3 did not reduce the color removal yields, but decolorization was delayed in the first SBR cycles.

[P-BB09]

Effect of engineered silver nanoparticles on the performance of aerobic granular sludge regarding the potential for abatement of textile wastewater toxicity

S. Sousa[1], M.S. Coelho[1], R.D.G. Franca[1], C.A. Viegas[1], H.M. Pinheiro[1], N.D. Lourenço[1,2,]*
[1] iBB – Institute for Bioengineering and Biosciences, Department of Bioengineering, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal; [2] UCIBIO, REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Campus de Caparica, 2829-516 Caparica, Portugal.
**nidia.lourenco@fct.unl.pt*

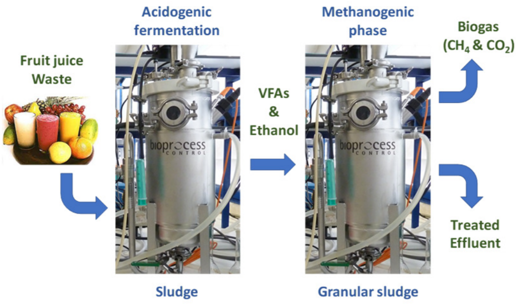


The present work aimed at examining the influence of silver nanoparticles (Ag NPs) on the performance of aerobic granular sludge (AGS) sequencing batch reactors (SBR) with respect to the potential detoxification of a simulated textile wastewater (TWW). Two types of TWW, with and without Ag NPs, both containing the azo dye Acid Red 14 (AR14), were fed in static conditions into two SBRs. Samples were collected from both SBRs at different cycle stages and assessed in terms of potential toxicity using yeast-based assays. Based on toxicity data over yeast growth, no relevant differences were found due to the presence of the Ag NPs during the SBR operation under the conditions tested. Measurement of possible changes in the transcript levels of two toxicity-indicator yeast genes brought about by the samples is in course. Data from the two types of bioassays at molecular and phenotypic levels will be integrated and discussed with respect to potential detoxification of the dye-laden TWW.

[P-BB10]

From fruit pulp waste to biogas: The assessment of substrate shifts on the performance of a two-stage anaerobic digestion system

S. Mateus[1], M. Carvalheira[1,], J. Cassidy[1], A. Oehmen[1], M.A.M. Reis[1]*
[1] UCIBIO, REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologias, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal
** mic16141@campus.fct.unl.pt*

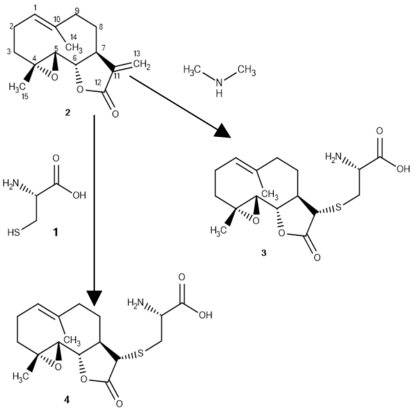


A two-stage anaerobic digestion system was operated treating different fruit pulp wastes (peach, raspberry and white guava) in a sequential operation in order to assess the effect of substrate shifts and operational conditions on the system's performance. Substrate shifts did not cause long-term instability issues and no evident association was found between operational condition changes and the effluent's composition and acidification degrees in the first stage. However, substrate composition seemed to affect the gas production and its composition in the first stage whereas it had no effect on the gas production and composition in the second stage. The biogas produced in the second stage was rich in methane (>75.9%) and high methane yields ($\approx$0.30 L_{CH4}/g_{COD}) and productivities (up to 2.13 L/(L.d)) were achieved throughout the operation. This process was shown to be robust in treating seasonal wastes from the fruit juice industry, suggesting that it could be applied in full scale.

[P-BB11]

NMR kinetic and cytotoxicity studies of sesquiterpene lactones

F. S. Mónica[*,1], *J.V. Barbosa*[1], *R.M.G. da Costa*[1,2], *I.C. Gonçalves*[3], *M.M.S.M. Bastos*[1]
[1] *LEPABE, Faculdade de Engenharia da Universidade do Porto, s/n, R. Dr. Roberto Frias, 4200-465 Porto, Portugal;*
[2] *Experimental Patology and Therapeutics group, CI-IPOP, IPO-Porto, R. Dr. A. Bernardino de Almeida, 4200-072, Porto, Portugal;*[3] *i3S - Instituto de Inovação e Investigação em Saúde, Universidade do Porto, Rua Alfredo Allen, 208, 4200-135 Porto, Portugal.*
* *monicafsilva@fe.up.pt*

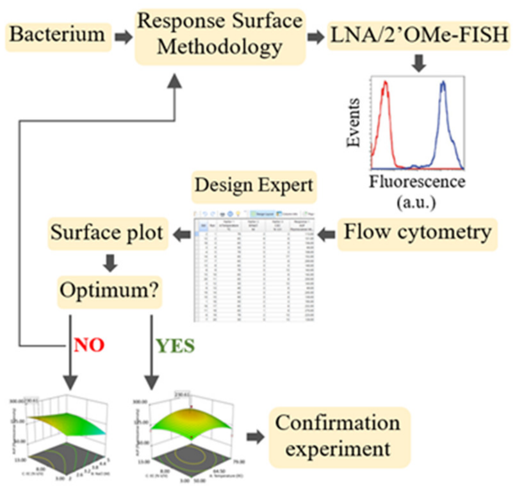


Sesquiterpene lactones (STL) are natural compounds that exert important biological activities by binding covalently to cysteine (CYS), 1, residues in target proteins. The aim of this study was to develop a method for studying the reaction between CYS and parthenolide (PT), 2, a natural STL with promising antineoplastic activity, and to study PT's cytotoxic activity against a tumor cell line. PT's derivative, dimethylaminoparthenolide (DMAPT), 3, is in cancer clinical trials. PT was mixed with CYS at an equimolar ratio and the reaction was followed over time by NMR spectroscopy. PT reacted very quickly with a half-live time lower than 5 min, following a second order kinetics and giving rise to parthenolide-cysteine adduct (PT-CYS), 4.The in vitro cytotoxicity of 2 and 3 against CaSki cells were compared. 2 was more active than 3, with IC50 of 5 and 12 µM, respectively. Further studies will clarify whether this difference in cytotoxicity is related to different CYS-binding potentials.

[P-BB12]

Optimizing locked nucleic acid/2'-O-methyl-RNA fluorescence *in situ* hybridization (LNA/2'OMe-FISH) for bacterial detection

A.S. Azevedo[1,2,3,4*], *I.M. de Sousa*[2], *R.Fernandes*[1,2,5], *N.F. Azevedo*[2], *C. Almeida*[5]
[1] *Centre of Biological Engineering, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal;* [2] *LEPABE - Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;* [3] *i3S Instituto de Investigação e Inovação em Saúde, Universidade do Porto, Porto, Portugal;* [4] *IPATIMUP, Institute of Molecular Pathology and Immunology of the University of Porto, Porto, Portugal;* [5] *Veterinary and Agrarian Investigation Institute (INIAV), Rua dos Lagidos, Lugar da Madalena, 4485-655 Vairão, Vila do Conde, Portugal.*
* *asazevedo@fe.up.pt*

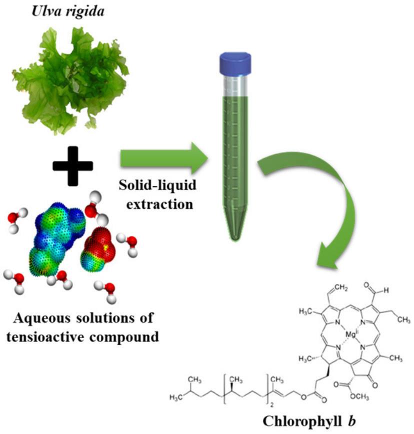


Despite the successful application of locked nucleic acid/2'-O-methyl-RNA fluorescence *in situ* hybridization (LNA/2'OMe-FISH) procedures for bacteria detection, there is a lack of knowledge on the properties that affect hybridization. Such information is crucial for the rational design of the protocols, especially in multiplex assays. Hence, this work aimed to evaluate the effect of 3 essential factors on the LNA/2'OMe hybridization step - hybridization temperature, NaCl concentration and type and concentration of denaturant (formamide, ethylene carbonate and urea). This optimization was performed for 3 Gram-negative bacteria (*Escherichia coli*, *Pseudomonas aeruginosa* and *Citrobacter freundii*) and 2 Gram-positive bacteria (*Enterococcus faecalis* and *Staphylococcus epidermidis*), employing the Response Surface Methodology and an Eubacteria probe. In general, it was observed that high NaCl concentrations (from 2 to 5M) are beneficial, regardless of denaturant. Urea, formamide and ethylene carbonate are suitable denaturants for FISH applications; but urea provides similar fluorescence signals among the different bacteria. Overall, the results indicate that 2 M of urea, 4 M of NaCl and 62 °C of hybridization temperature would be a proper starting point for multiplex LNA/2'OMe-FISH procedures.

[P-BB13]

Aqueous solutions of tensioactive ionic liquids: alternative solvents in the chlorophyll extraction from green macroalgae

M. Martins[1,], A.P.M. Fernandes[1], J.A.P. Coutinho[1], S.P.M. Ventura[1]*
[1]CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.
** margaridamartins@ua.pt*

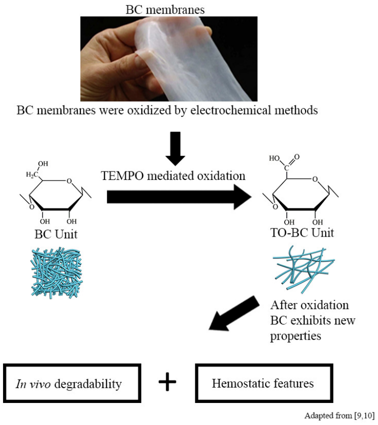


Recently, the interest in the products obtained from natural sources has grown in relation to synthetic products. Thus, industry and academia have given particular attention to products derived from natural sources. Some of these interesting compounds can be found in abundance in green algae. Chlorophylls appear as such an example. However, the conventional extraction methodologies are based on organic solvents, which present a low selectivity and are often recognized by negatively environmental impacts. In this work, a set of experimental operational conditions were studied in order to develop an efficient method to extract efficiently chlorophyll from fresh *Ulva rigida*. Aqueous solutions of tensioactive ionic liquids and surfactants were tested, and the extraction conditions evaluated for the best solvents selected. After, studies on environmental and economic impacts were carried out and compared with the conventional methodology.

[P-BB15]

The potential of bacterial cellulose as hemostatic material

E.C. Queirós[1], S. Pinheiro[1], P. Parpot[1,2,], M. Gama[1]
[1] CEB-Centre of Biological Engineering, University of Minho, 4710-057 Braga, Portugal; [2] CQUM – Centre of Chemistry, University of Minho, 4710-057 Braga Portugal;
** eugeniaqueiros@ceb.uminho.pt*

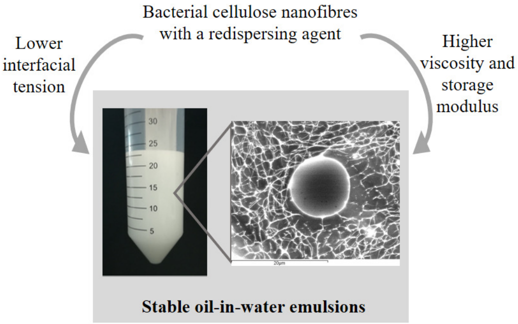


Bacterial cellulose (BC) produced by *Komagataeibacter* exhibits suitable properties for biomedical applications. However, BC is not biodegradable being mandatory its chemical modification by oxidative methods, making it biodegradable when implanted in the human body. Tetramethylpiperidine-1-oxyl (TEMPO) radical has been applied to oxidize cellulose since allows the selective oxidation of the primary hydroxyl group at C6 into carboxyl groups. Thus, we aimed at developing a hemostatic material based on the oxidized BC. The oxidation of BC was achieved through electrochemical methods using TEMPO. The oxidation of the hydroxyl groups was analysed by FT-IR and the selective oxidation of C6 was confirmed by ^{13}C-NMR. SEM was used to assess the surface morphology of BC membranes and the *in vitro* degradation was investigated in ultra-pure water. The hemostatic behavior was evaluated using whole blood coagulation tests.

[P-BB16]

Bacterial cellulose as a stabilizer for oil-in-water emulsions

D. Martins[1,*], A. Fontão[2], F. Dourado[1], M.. Gama[1]
[1] CEB- Centre of Biological Engineeing, Universidade do Minho, 4710-057 Braga, Portugal; [2] Satisfibre S.A., SpinPark - Centro de Incubação de Base Tecnológica, Zona Industrial da Gandra, S. Claudio do Barco, 4805-017 Guimarães, Portugal
*dsr.martins@ceb.uminho.pt

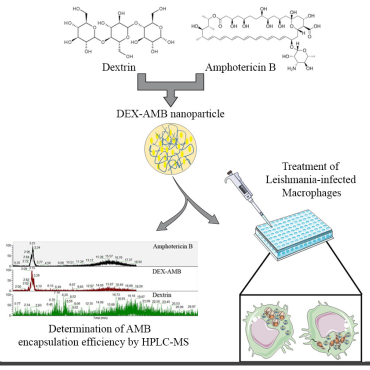


Cellulose is the most abundant biopolymer on earth, being plant sources the most significant. This material has been showing increasing applications in many fields: biomedicine, food, cosmetics, electronics, composite materials, among others. Cellulose from bacterial sources is a prominent alternative to the already marketed celluloses, being more pure, crystalline, having nanoscale fibres and excellent mechanical properties. One of the many uses of cellulose, in its various forms, is the stabilization of heterogeneous systems – more specifically, the stabilization of oil-in-water emulsions. In this work, bacterial cellulose's potential as a stabilizer for Pickering emulsions was assessed. A model system of an isohexadecane-in-water emulsion was studied in detail. A dry bacterial cellulose formulation was able to lower the interfacial tension between the immiscible phases. Emulsions prepared with this formulation showed good stability over time and desired rheological behavior.

[P-BB17]

Development of a water-soluble dextrin-amphotericin B conjugate for the treatment of Leishmaniasis

J. Fidalgo[1, 2 *], R. Silva-Carvalho[1*], S. Leal[1], T. Cruz[2], AM. Tomás[2], P. Parpot[1, 3], M. Gama[1]
[1] CEB - Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal; [2] I3S - Instituto de Investigação e Inovação em Saúde, Universidade do Porto and IBMC - Instituto de Biologia Molecular e Celular, Universidade do Porto, Porto, Portugal; [3] Centre of Chemistry, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal.
* remanuelcarvalho@gmail.com

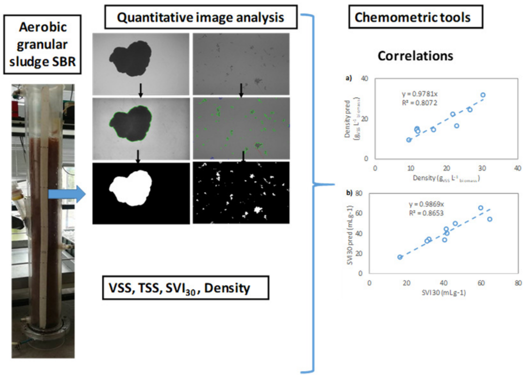


Leishmaniasis is a life-threatening disease with a worldwide distribution and a huge impact especially in immunocompromised patients. Nowadays, the use of amphotericin B, an antifungal agent, or other marketed strategies to overcome this disease exhibit major clinical limitations. Thus, other strategies have been pursued to achieve better clinical treatments and decrease toxicity. In this work, a promising conjugate based on dextrin and amphotericin B was developed. An HPLC-MS detection method was also developed in order to determine the amphotericin B concentration and the encapsulation efficiency. This water-soluble polymer-drug conjugate has shown promising effects against axenic cultures of *Leishmania amazonensis* parasite and infected macrophages, without being cytotoxic to the latter.

[P-BB18]

Density and sludge volume index estimation in mature aerobic granular sludge by quantitative image analysis and chemometric tools

C. Leal[1,], A. Val del Río[1], A. Zlatkova[1], B. Araújo[1], D.P. Mesquita[1], A.L. Amaral[1,2], E.C. Ferreira[1]*
[1] Centre of Biological Engineering, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal
[2] Instituto Politécnico de Coimbra, ISEC, Rua Pedro Nunes, Quinta da Nora, 3030-199 Coimbra, Portugal.
** cristiano.leal@ceb.uminho.pt*

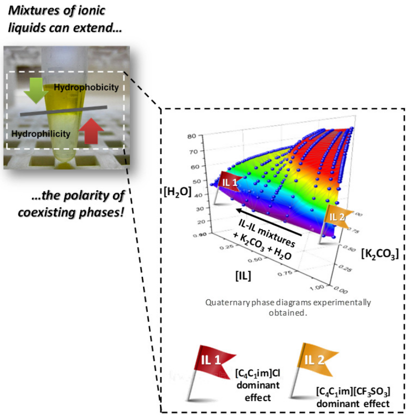


Quantitative image analysis (QIA) has already been applied for activated sludge dysfunctions and anaerobic granular sludge processes elucidation and its application to aerobic granular sludge characterization is considered of major interest. In this work, a sequencing batch reactor (SBR) was operated using mature aerobic granular sludge for pharmacologically active compounds (PAC) removal. The physicochemical parameters (total and volatile suspended solids, sludge volume index and density), prior to the introduction of PAC, were determined by analytical methods. The mature aerobic granular and suspended sludge morphological and structural parameters were established by QIA. The objective of this study is to characterize this mature granular sludge by QIA, and establish relationships for physicochemical parameters (aggregates density and SVI30) with QIA data using chemometric tools. Indeed, relevant relationships could be found for both density (R^2 of 0.81) and SVI_{30} (R^2 of 0.87).

[P-BB19]

Aqueous biphasic systems composed of mixtures of ionic liquids: Phase diagrams and separation performance

T.B.V. Dinis[1,], H. Passos[1], M. G. Freire, J. A.P. Coutinho[1]*
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal.
** tbdinis@ua.pt*

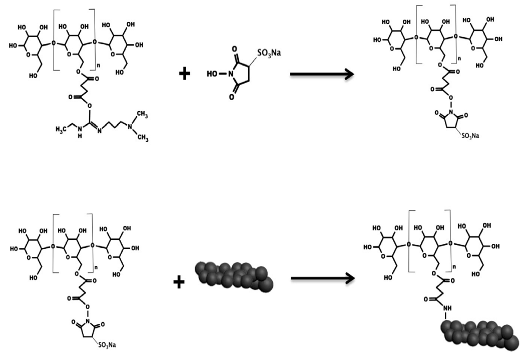


With the aim of manipulating the aqueous biphasic systems (ABS) ability to undergo liquid-liquid demixing and the respective coexisting phases' polarities, ABS formed by mixtures of two ionic liquids (ILs) with a common cation and different anions, water, and a salt were investigated. The respective liquid-liquid (pseudo-quaternary) phase diagrams were determined and characterized at 298.15 K for these systems at different IL mole fractions. Their extraction performance was then evaluated for a series of biocompounds to infer the tunability of these systems selectivity by using IL mixtures at different mole fractions. The results obtained suggest that each IL has a region where its effect to form two-phase systems prevails over the other, i.e. each IL is individually salted-out by the inorganic salt. This behavior also allows the tuning of the ABS coexisting phases properties, which can be advantageous for the development of effective separation platforms in biotechnological processes.

[P-BB20]

Dextrin: a platform for the development of drug delivery systems

A. Machado[1,*], J. Martins[2], J.E. Pereira[3], M. Gama[1]
[1] *CEB - Centre of Biological Engineering, University of Minho, Campus de Gualtar, Braga, Portugal;* [2] *Department of Chemistry, University of Minho, Campus de Gualtar, Braga, Portugal;* [3] *CECAV - Centre of Animal and Veterinary Science, University of Trás-os-Montes and Alto Douro, Vila Real, Portugal.*
* *xana.meira.machado@gmail.com*

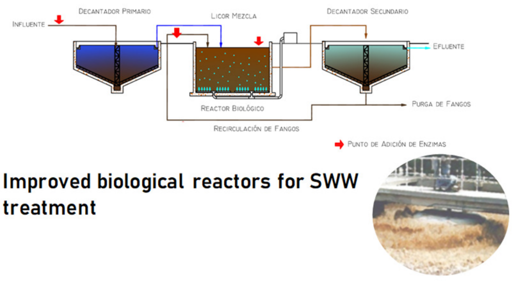


Dextrin is a biocompatible polysaccharide that can be suited for the conjugation with bioactive agents while enabling controlled release at the target site. LLKKK18, an LL37 human cathelicidin analog, has been engineered to enhance antimicrobial properties and decrease toxicity. In this work, chemically modified dextrin bearing a carboxylic group has been produced to allow the conjugation with LLKKK18 for the treatment of osteomyelitis. FT-IR spectra confirmed dextrin modification while maximum degradability was achieved after approximately 2h. A batch of 30% mol modification was used to conjugate with LLKKK18 and incubated *in vitro* with *Staphylococcus aureus*. Conjugates incubated with α-amylase were more effective in killing bacteria when compared to conjugates with intact bonds, emphasizing the protective effect of dextrin and indicating a controlled peptide release.

[P-BB21]

Application of enzyme technology in the improvement of wastewater treatment systems

C. Aragon[1,*], A. Real[1], I. Martin[1], K. Fahd[1], J. Parrado[2], P. Caballero[2]
[1] *Fundacion CENTA. Autovia Sevilla-Huelva (A49) km 28. 41820. Carrion de los Céspedes, Spain;* [2] *Department of Biochemical and Molecular Biology, Faculty of Pharmacy, University of Seville, Spain.*
* *caragon@centa.es*

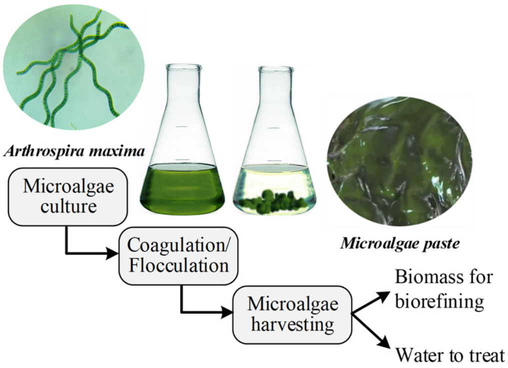


Urban wastewater treatment is commonly based on biological processes, and therefore its success depends on the uptake of contaminants by the microorganisms present in the treatment units. Many of the conventional treatment systems are inefficient and the final effluent does not meet the emission limit values required for the discharge to the environment (D91/271/EEC) or its further reuse, showing low rate of degradation of organic matter (presence of recalcitrant components). Therefore, it is crucial to develop technological innovations to make the treatment of wastewater an efficient and effective process. In this sense, the use of enzymatic biocatalysts could lead to a significant improvement in the performance of wastewater treatment plants. In this work, batch tests to assess the effect of enzymes dosage to an activated sludge system are proposed. Although, initially, no effect is observed on the removal of organic matter, a reduction in the sewage sludge production is detected.

[P-BB22]

Harvesting of *Arthrospira maxima* by coagulation/ flocculation

N.S. Caetano[1,2*], A.A. Martins[1], M. Gorgich[1], D.M.R. Gutiérrez[1], L.J.S. Ribeiro[2], T.M. Mata[1]
[1] LEPABE, Faculty of Engineering University of Porto, R. Dr. Roberto Frias, 4200-465 Porto, Portugal; [2] CIETI/ISEP (School of Engineering), Polytechnic of Porto, R. Dr. António Bernardino de Almeida 431, 4249-015 Porto, Portugal
* nsc@isep.ipp.pt

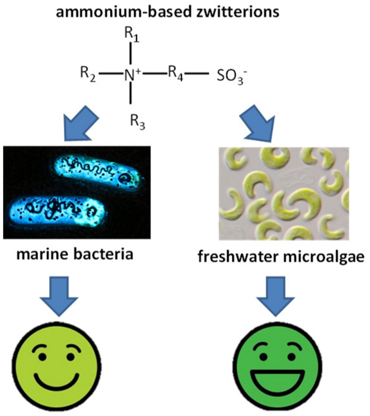


Biodiesel production from microalgae still faces big challenges to achieve a commercial and profitable production, in particular due to harvesting, one of the most energy intensive steps of the whole process. On the other hand, use of complex chemicals may pose additional problems to the later water disposal. Thus, in this study, the effectiveness of coagulation-flocculation methods induced only by pH variation and by the addition of flocculants were evaluated for *Arthrospira maxima*. Results show that *Arthrospira maxima* can be effectively harvested by increasing the pH over 10 with NaOH or by adding calcium chloride as flocculant with a concentration of about 0.2-0.3 g/L and a 1:30 volume ratio of $CaCl_2$/microalgae culture. Other chemicals, such as NH_3, $Al_2(SO_4)_3$, Na_3PO_4, HCl and $MgSO_4$ have also been tested but without positive results.

[P-BB23]

Toxicity of ammonium-based zwitterions to aquatic organisms

F. Jesus[1,*], H. Passos[2], F. Gonçalves[1], J.A.P. Coutinho[2], S.P.M. Ventura[2]
[1] Department of Biology & CESAM, University of Aveiro, 3810-193 Aveiro, Portugal; [2] CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.
* fatima.jesus@ua.pt

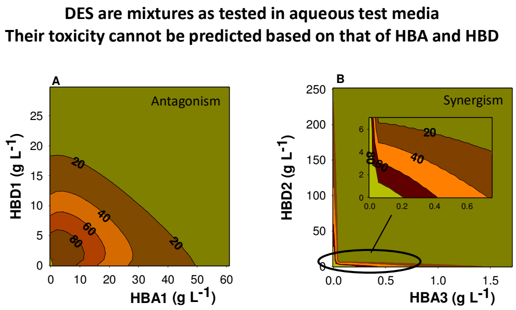


Our goal was to assess the toxicity of four ammonium-based zwitterions (ZIs) with different alkyl side chain lengths to a marine organism (bacterium *Vibrio fischeri*) and a freshwater organism (microalga *Raphidocelis subcapitata*). None of the tested ZIs was hazardous to these species. For both organisms, the increase of the ZI alkyl chain resulted in higher toxicity, which is likely related to the ZIs hydrophobicity. The toxicity was higher for *V. fischeri* than for *R. subcapitata*. For the algae, the toxicity varied widely among the ZIs, with a maximum variation of 17-fold. Concerning the bacteria, the toxicity varied slightly, with a maximum variation of 3-fold. This, allied to the fact that ZI's were more toxic to the marine than to the freshwater species, raises concern about the effects of ZIs to marine organisms and highlights the importance on screening their toxicity. Moreover, the results suggest that the toxicity tests should not be performed exclusively with freshwater species.

[P-BB24]

Unraveling the ecotoxicity of deep eutectic solvents using the mixture toxicity theory

F. Jesus[1,*], *I.P.E. Macário*[1], *J.L. Pereira*[1], *S.P.M. Ventura*[2], *A.M.M. Gonçalves*[1,3], *J.A.P. Coutinho*[2], *F.J.M. Gonçalves*[1]
[1]*Department of Biology & CESAM, University of Aveiro, 3810-193 Aveiro, Portugal;* [2]*CICECO - Aveiro Institute of Materials & Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;*[3] *MARE, Department of Life Sciences, Faculty of Science and Technology, University of Coimbra, 3004-517 Coimbra, Portugal.*
** fatima.jesus@ua.pt*

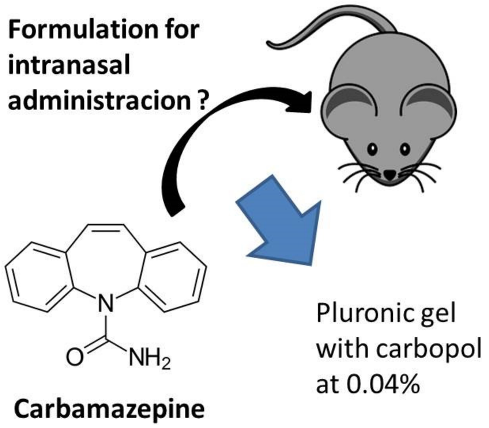


This study aims to assess the ecotoxicological profile of deep eutectic solvents (DES) based on three quaternary ammonium salts as hydrogen bond acceptors (HBA) combined with two hydrogen bond donors (HBD), through the Microtox® Acute Toxicity Test. Concentration addition (CA) and independent action (IA) with deviations were fitted to the experimental data. DES toxicity followed the same trend as the salts, highlighting the role of HBAs on DES toxicity. Antagonism was observed for HBA1-based DES and synergism for HBA3-based DES. As demonstrated here for the first time, the application of the mixture toxicity models represents a breakthrough in the problematic of assessing DES toxicity, given the potentially countless number of DES that can be created with the same starting materials. The graphical representation of the response curves will allow the prediction of DES toxicity (varying ratios of the same HBA:HBD) without having to test them all experimentally.

[P-BB25]

The contribution of carbomer in pluronic-based thermoreversible gels of carbamazepine.

J. Ferreira[1,2*], *P.C.Pires*[1,2], *G. Alves*[1,2], *A. O. Santos*[1,2]
[1] *Health Sciences Research Centre (CICS-UBI), University of Beira Interior, Av. Infante D. Henrique, 6200-506 Covilhã, Portugal;* [2] *Faculty of Health Sciences, University of Beira Interior, Av. Infante D. Henrique, 6200-506 Covilhã, Portugal.*
** joana_gferreira@hotmail.com*

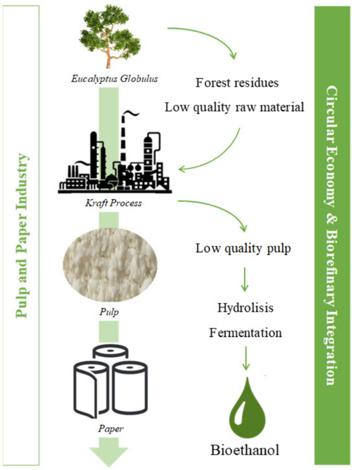


Pluronic (poloxamer) and Carbopol (carbomer) are polymers that have been used to obtain thermoreversible gels for intranasal delivery of many drugs, including carbamazepine (1). To evaluate the influence of Carbopol 974P in formulation's viscosity, drug precipitation and in-vitro release of carbamazepine, four thermoreversible gels were prepared with Pluronic F-127 at 15% (m/m) and Carbopol at 0.17% (1), 0.08%, 0.04% or 0% (m/m). Viscosity was measured using a cone-plate rheometer. In-vitro release of carbamazepine was tested in horizontal Ussing Chambers. Formulations with Carbopol permitted the incorporation of a higher percentage of drug in comparison with the formulation without this polymer. The formulations with lower viscosity, at 0% and 0.04% Carbopol, showed higher rate of drug release. Carbopol at 0.04% can prevent short-term drug precipitation, allowing higher drug strength, without inhibiting drug release, and without changing the viscosity of the poloxamer formulation.

[P-BB26]

Production of second generation bioethanol from unbleached Kraft pulp of *Eucalyptus globulus*

M.S.T. Amândio[1,*], *R.H.R.Branco*[1], *L.S. Serafim*[1], *A.M.R.B. Xavier*[1]
[1] *CICECO – Aveiro Institute of Materials, Departamento de Química, Universidade de Aveiro, Aveiro, Portugal.*
* *m.amandio@ua.pt*

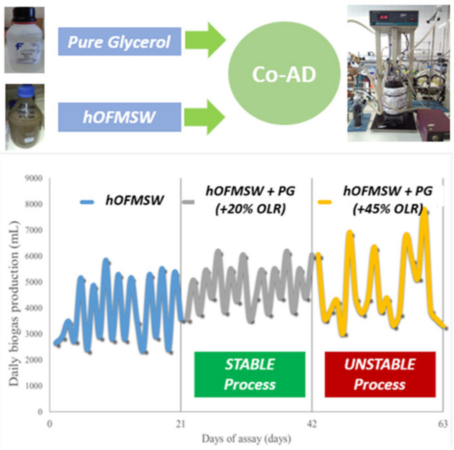


Bioethanol is the biofuel produced at the largest scale. However, since it is mainly obtained from agricultural crops that interferes with the food chain, its sustainability has been questioned [1]. In this regard, the production of bioethanol from lignocellulosic biomass (LCB) is a promising alternative [2]. Despite all the advantages, its large-scale production is not yet implemented since it requires a high capital investment [3]. The pulp and paper industry contributes significantly to the Portuguese economy [4]. Kraft pulping allows for the removal of lignin from wood and is the most widely used pulping process. Its use as a pretreatment of forest residues before their conversion into bioethanol LCB would be advantageous [5]. It can be integrated in a LCB biorefinery following the circular economy concept. The aim of this work was the study of the production of bioethanol from unbleached Kraft pulps of *Eucalyptus globulus*.

[P-BB27]

Effect of glycerol on the anaerobic co-digestion of the organic fraction of municipal solid wastes

*A. Deodato, E. Surra, N. Lapa**
LAQV-REQUIMTE, Departamento de Ciências e Tecnologia da Biomassa, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal.
** ncsn@fct.unl.pt*

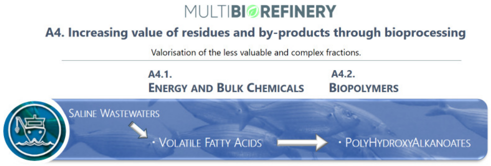


The Anaerobic co-Digestion (AcoD) of the Organic Fraction of Municipal Solid Wastes (OFMSW) with other substrates is one of the most efficient processes to overcome the Carbon limitation of OFMSW. Anaerobic Digestion (AD) and AcoD of a hydrolysed OFMSW (hOFMSW) with Pure Glycerol (PG) was tested under three different organic load rates (OLR): AD with hOFMSW = 2.92 g COD/L.d; AcoD with PG = 20% and 45% increases of OLR when compared to the assay with hOFMSW alone. In AcoD assays, it was possible to achieve, on average, an increase of 20% in biogas daily production when compared to hOFMSW alone. Although CO_2 and H_2S have increased with the addition of PG, biogas and methane yields showed no significant variation from the AD assay to the AcoD assays. An increase of 20% OLR with PG has stabilised the biogas daily production, while an increase of 45% OLR resulted in an unstable process with H_2S reaching the highest concentration (higher than 1500 ppmv).

[P-BB28]

Valorise saline wastewaters through the production of polyhydroxyalkanoates (PHA) biopolymers by mixed microbial consortia (MMC)

BC. Marreiros[1], S. Mateus[1], C.S.S. Oliveira[1,], M.A.M. Reis[1]*
[1] UCIBIO-REQUIMTE, Dep. Chemistry, Faculty of Science and Technology, Universidade NOVA de Lisboa,
2829-516 Caparica, Portugal
**css.oliveira@fct.unl.pt*

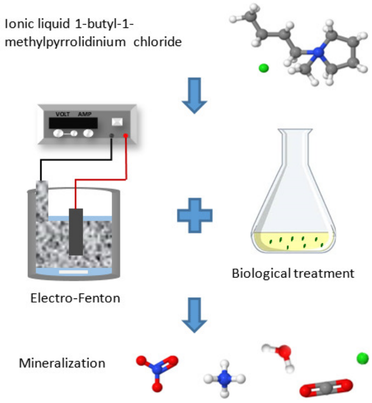


PHAs (Polyhydroxyalkanoates) are microbial polyesters that can be used to produce bioplastics. A cost-effective and eco-friendly approach to produce PHAs is based on Mixed Microbial Consortia (MMC) processes and the use of waste or industry by-products as feedstocks. Within the scope of MultiBiorefinery project, a process to valorise industrial saline wastewaters through the production of PHA biopolymers by MMC is on development. A stable PHA-producing halotolerant MMC-based process was effectively established from a salt non-acclimatised inoculum, applying a successful start-up strategy and using a synthetic Volatile Fatty Acids (VFAs) mixture with 20 gNaCl.L^{-1}. The following step consists in validating the developed star-up strategy to real industrial wastes, salted cheese whey and fish canning residues.

[P-BB29]

Bio-electro-Fenton hybrid process as a plausible methodology for the degradation of ionic liquids

M. Arellano[1,2,], N. Oturan[1], M. A. Sanromán[2], M. Pazos[2], M. A. Oturan[1]*
[1] Laboratoire Géomatériaux et Environnement (LGE), Université Paris-Est, EA 4508, UPEM, 5 Bd Descartes, 77454, Marne-la-Vallée, Cedex 2, France; [2] Department of Chemical Engineering, University of Vigo, Isaac Newton Building, Campus As Lagoas-Marcosende, 36310 Vigo, Spain.
**marellano@uvigo.es*

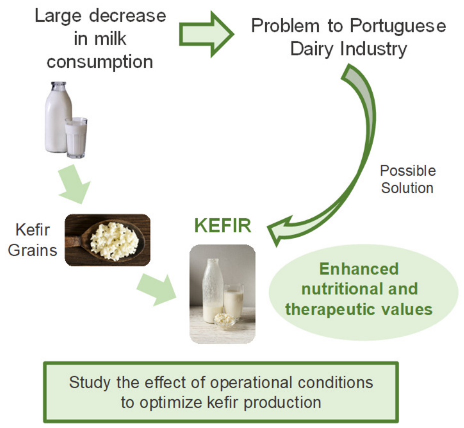


In the present study, the degradation of the ionic liquid 1-butyl-1-methylpyrrolidinium chloride has been carried out through a system combining an electro-Fenton pre-treatment and a biological post-treatment. The effect of the key parameters was evaluated, since the effect of the iron dosage (0.1-0.2 mM), the applied current (50-1000 mA) and the ionic liquid initial concentration (0.075-2.5 mM), using boron doped diamond (BDD) and sub-stoichiometric titanium oxide anodes. A total organic carbon decay of 98% was obtained with a dosage of iron 0.1 mM, 1000 mA current and a concentration of ionic liquid 0.15 mM. Before coupling the biological process, the average oxidation state and carbon oxidation state were calculated to evaluate the biodegradability of the solution. Based on the results, after an electro-Fenton treatment of 30 min, the biological process was attached. The efficiency of the system was followed by the total organic carbon and released carboxylic acids measurements.

[P-BB30]

Study of kefir production

J. Anjos[1,*], *A. Lei*[1], *L.S. Serafim*[1], *A.M.R.B. Xavier*[1]
[1] *CICECO – Aveiro Institute of Materials, Departamento de Química, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal;*
** joshua@ua.pt*

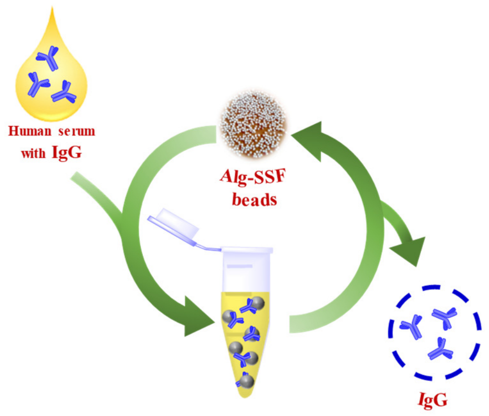


Kefir is a fermented milk beverage with unique sensory properties and high nutritional and therapeutic values. Currently, there is an increase in its consumption and manufacture in many countries, however, in Portugal, only recently this beverage has started to be produced industrially. Therefore, a detailed study of kefir production should be done to help expanding the implementation of kefir industrial process in Portugal. In this work, several fermentation conditions were studied and compared, concerning pH values, lactose, lactic and acetic acids, and ethanol concentrations: initial kefir grains mass concentration (3 %, 6 % and 9 % (m/v)), initial milk volume (100 and 200 mL), temperature (28 ºC and room temperature) and agitation rate (0, 60 and 180 rpm). The best conditions for kefir production were achieved with 9 % (m/v) of kefir grains, 200 mL of milk volume, 28 ºC and without agitation, allowing the production of kefir in approximately 8 h.

[P-BB31]

IgG purification with alginate-protein fibril composites

M. Sharma[1], M. C. Neves[1]*, A. P. M. Tavares[1], D. Mondal[2], N. Singh[3], K. Prasad[3], M. G. Freire[1]
[1]*Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193, Aveiro, Portugal;* [2]*Centre for Nano & Materials Sciences, Jain University, Kanakpura, Ramanagaram, Bangalore, 562112, Karnataka, India;* [3]*Natural Products & Green Chemistry Division, CSIR-Central Salt & Marine Chemicals Research Institute, Bhavnagar, 364002, Gujarat, India.*
**mcneves@ua.pt*

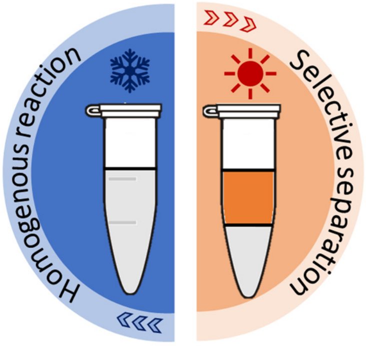


Significant advances of therapeutics action have been observed using biopharmaceuticals, namely with antibodies such as Immunoglobulin G (IgG). However, the purification of antibodies for therapeutic applications requires the use of highly selective and robust technologies, which are highly expensive. In this work, alginate fibril composites were prepared, characterized and applied for the IgG purification from human serum. Several operating conditions were optimized: pH, adsorption time and serum concentration, aiming at improving the IgG recovery and purity. After the adsorption step, the IgG desorption and recovery were addressed. IgG with a purity of 80% and a recovery yield of 41% was obtained. The reuse of the composite materials was also evaluated and no loss in their adsorption performance was observed. This work demonstrates the potential of seaweed polysaccharide-based materials for the purification of high value (bio)molecules.

[P-BB32]

Integrated biocatalytic processes by using thermoreversible aqueous biphasic systems

A.M. Ferreira,[1] H. Passos, [1] A. Okafuji,[2] A.P.M. Tavares,[1] H. Ohno,[2] M.G. Freire[1], J.A.P. Coutinho[1]*
[1]CICECO – Aveiro Institute of Materials, Chemistry Department, University of Aveiro, Portugal;[2]Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology, Koganei, Tokyo, Japan.
** aptavares@ua.pt*

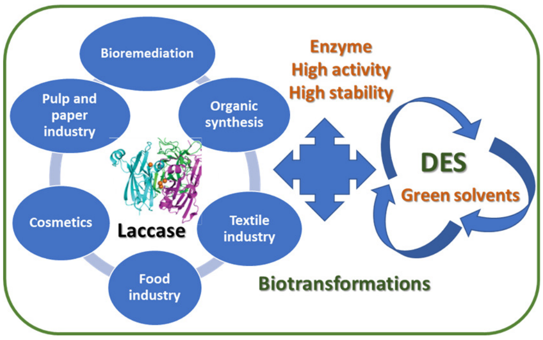


Thermoreversible aqueous biphasic systems (ABS) composed of ammonium-based zwitterions (ZIs) and polymers are here disclosed to act as integrated bioreaction-separation processes. The biocatalytic reaction involving laccase occurs in homogeneous media, after which small changes in temperature induce the formation of two phases and the complete separation of the enzyme from the products in a single-step. These systems also allow the recovery and reuse of the enzyme, along with the ZI-rich phase, contributing towards the development of sustainable biocatalytic processes.

[P-BB33]

Activation of laccase in the presence of natural deep eutectic solvents

M.L. Toledo[1,2], M.M. Pereira[1], M.G. Freire[1], J.A.P. Coutinho[1], J.P.A. Silva[2], A.P.M. Tavares[1,]*
[1] CICECO – Aveiro Institute of Materials, Chemistry Department, University of Aveiro, 3810-193 Aveiro, Portugal; [2] Engineering School of Lorena, Chemical Engineering Department, University of São Paulo, 12602-810, Lorena, São Paulo, Brazil.
** aptavares@ua.pt*

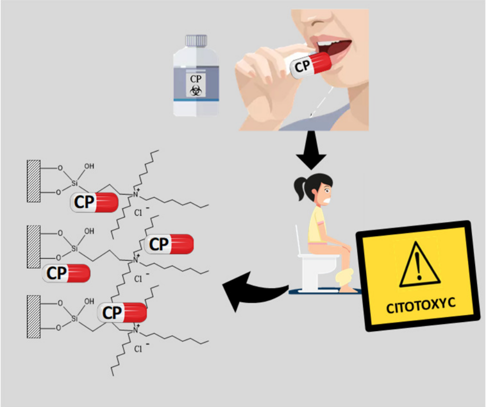


Aiming the development of new strategies for biocatalytic reactions, novel eco-friendly solvents, such as deep eutectic solvents (DES), have been emerged as an attractive new reaction medium. DES display many advantages in comparison to the traditional organic solvents due to their high biodegradability, low toxicity and simple preparation. Traditionally, enzymatic catalysis has been performed in water or organic solvents. However, the presence of organic solvents could promote enzyme denaturation and/or deactivation. The present work aims to evaluate DES as potential co-solvent in biocatalytic reactions. Laccase was used as a model enzyme and its catalytic performance was determined in DES. Several DES constituted by cholines/polyols and betaine/polyols were tested. According to results, laccase activity in presence of DES increases 1.7 times (comparing to control – without DES) showing the potential ability of DES composed of biocompatible and non-toxic natural compounds.

[P-BB34]

Supported ionic liquids for the removal of cyclophosphamide from aqueous solutions

B. Rocha, M. C. Neves, A.C. Sousa, T. Trindade, M. G. Freire*
Department of Chemistry and CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal
** beatriz.rocha@ua.pt*

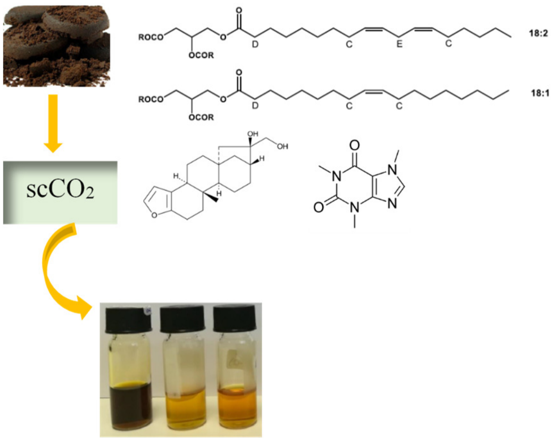


The incidence of cancer is increasing and with it also the consumption of anti-cancer drugs. As with other drugs, these compounds are not completely metabolized and are excreted through the urine, ultimately reaching waste water treatment plants (WWTPs). Anti-cancer drugs are emerging pollutants, reinforcing the need for developing effective treatment or removal strategies. This work aims to contribute to the development of an efficient material for the removal of anti-cancer drugs, namely cyclophosphamide (CP), from urine. This strategy envisages the removal of anti-cancer drugs at the entrance point to avoid the contamination of water streams. To this end, six supported ionic liquids (SILs) were synthesized and characterized. A preliminary study was carried out to address the efficiency of these materials for the removal of CP from aqueous solutions. Kinetic and adsorption isotherms were determined for the best materials, and future studies will be carried out with urine samples.

[P-BB35]

Valorization of spent coffee grounds with supercritical fluids

J.P. Coelho[1,2,], F. Campos[1], M. P. Robalo[1,2], G.St. Cholakov[3], S. Boyadzieva[4], R. P. Stateva[4]*
[1]Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, 1959-007 Lisboa, Portugal; [2] Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, 1049-001, Lisboa, Portugal; [3] University of Chemical Technology and Metallurgy, 1756 Sofia, Bulgaria; [4] Institute of Chemical Engineering, Bulgarian Academy of Sciences, 1113, Sofia, Bulgaria.
** jcoelho@deq.isel.ipl.pt*

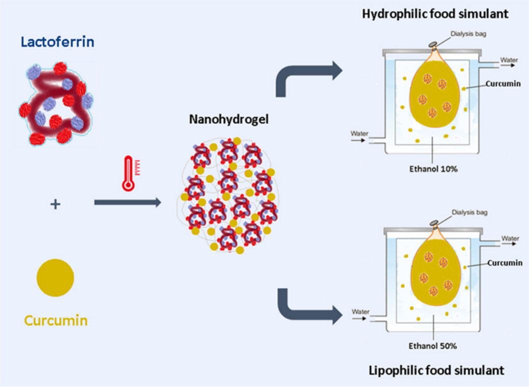


Spent coffee grounds (SCGs) are a potential sustainable source of high value added compounds. Extractions with pure supercritical CO_2 ($scCO_2$) and $scCO_2$+co-solvents (10% ethanol, 10% *i*-propanol and 5% ethyl lactate) of SCGs were used for valorization of the waste biomass. Conditions for highest yields (30 MPa and 323 K for extractions with co-solvents and 40 MPa and 313 K - for those with pure $scCO_2$) were identified and applied for comparison. The results, in terms of global yield and elemental composition, were compared with those achieved by pure $scCO_2$ and by conventional Soxhlet extraction with *n*-hexane. The highest yield of 12.3%was obtained with $scCO_2$+5% ethyl lactate, yields of (10.1 to 12) % - with the rest of the extractions, and 10.4 %-by the Soxhlet extraction. Quantitative identification of diterpens in the extracts was carried out by H-NMR. Elemental analysis provided useful information for the application of SCGs products, obtained with the tested extraction technologies.

[P-BB36]

Behavior of lactoferrin nanohydrogels incorporating curcumin as model compound into food simulants

J.F. Araújo[1,2,*], *A.I. Bourbon*[3], *A.A. Vicente*[2], *P.Coutinho*[1], *O.L. Ramos*[2]
[1] Escola de Ciências, Campus de Gualtar Braga, Portugal; [2] Center of Biological Engineering of University of Minho, Campus de Gualtar, Braga, Portugal; [3] International Iberian Nanotechnology Laboratory, Av. Mestre José Veiga, Braga, Portugal.
** pg32656@alunos.uminho.pt*

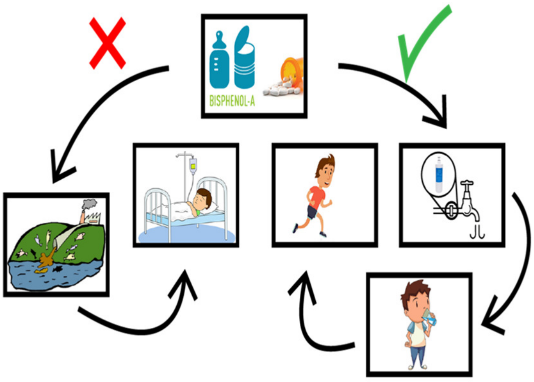


In this study, a lactoferrin (LF) nanohydrogel was developed to encapsulate curcumin as a nutraceutical model aiming at its behavior evaluation. The release kinetics of curcumin from LF nanohydrogels were also performed when added to food simulants (hydrophilic medium_ethanol 10 % and lipophilic medium_ethanol 50 %) (According to the COMMISSION REGULATION EU No 10/2011). For this purpose, the protein nanohydrogel isolated and loaded with curcumin was comprehensively characterized resorting to several techniques such as dynamic light scattering (DLS), fluorescence measurements, circular dichroism (CD), Fourier-transform infrared spectroscopy (FTIR) and transmission electron microscopy (TEM). This system was able to associate curcumin at 80 µg/mL with a remarkable efficiency of ~90 % and loading capacity of ~3 %. LF nanohydrogel showed higher release rates of curcumin in a lipophilic food simulant (after ~10 hours) in comparison with a hydrophilic one (after ~25 hours).

[P-BB37]

Supported ionic liquids as efficient adsorbents for the removal of bisphenol A

G. Lobo-Sousa*, M. C. Neves, A. C. Sousa, T. Trindade, M. G. Freire
Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal
** guilherme.lobo@ua.pt*



One of the main concerns in human health and environment is the contamination of water by various pollutants, such as anti-inflammatory drugs, endocrine disrupters (e.g. bisphenol A, BPA), antibiotics, analgesics. These compounds are widely used but are not efficiently removed or treated at wastewater treatment plants (WWTPs). BPA is an ubiquitous compound present in consumer products that ending in WWTPs. BPA is considered an endocrine disruptor with implications in ecosystems' and public health. Several techniques have been proposed to remove BPA from WWTPs but none are efficient. Therefore, there is an urgent need to develop cost-effective techniques to remove endocrine disruptors such as BPA from WWTPs, and for which supported ionic liquid phases (SILPs) can be used as an alternative approach. SILPs allow an easy manipulation of their chemical structure, and as such their chemical properties can be adjusted to improve their removal performance.

[P-BB38]

Comparative evaluation of the efficiency of acid pretreatment in energy cane in relation to sugarcane bagasse

R.S. Alves[1,*], *Ê.d.S. Araujo*[1], *S.M.N. de Assumpção*[2], *L.M A. Campos*[1], *L.A.M. Pontes*[2]
[1]*Catalise e Ambiente (CATAM), Universidade Salvador (UNIFACS), Av. Cardeal da Silva, 132, Federação, Salvador, Brazil;* [2] *Universidade Federal da Bahia (UFBA), R. Prof. Aristídes Novis, 2, Federação, Salvador, Brazil;*
**rebecasalves@hotmail.com*

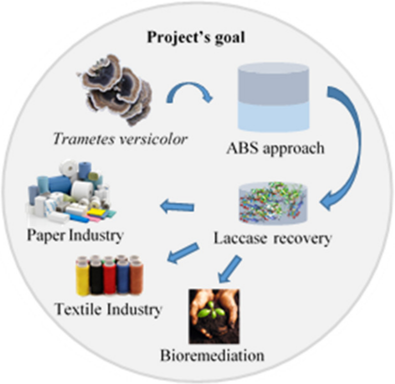
Several studies have been published regarding pretreatments for the optimization of the production process of biofuels from sugarcane. Pretreatments performed with dilute acids and alkaline substances are considered the most efficient in rupturing the rigid structure of the lignocellulosic material. Research on the hybrid has been intensified due to the possibility of increasing the energy matrix. Due to its high fiber content and low sucrose content, energy-cane proved itself as a superior material for biofuels. Furthermore, the hybrid is more adaptable to climate variations and has a higher yield per hectare production. In addition, studies estimate that the production of ethanol from energy-cane has the potential to produce approximately twice as much ethanol as sugarcane. In this context, the present study evaluates the efficiency of the pretreatment stage of energy-cane using dilute sulfuric and phosphoric acids to remove hemicellulose compared to the results of sugarcane bagasse.

[P-BB39]

Extraction of laccase from *Trametes versicolor* growth media using aqueous biphasic systems

M.E. Rosa[1], *C.M. S. S. Neves*[1], *A.M. R. B. Xavier*[1], *A.P.M. Tavares*[1], *M.G. Freire*[1]

[1]*CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.*
** marguerita.rosa@ua.pt*

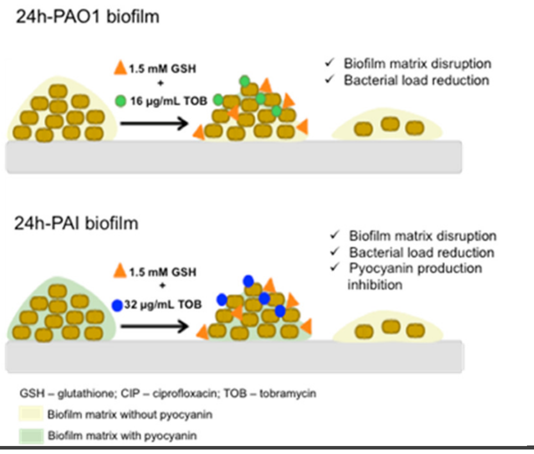


Biocompounds extracted and recovered from living organisms are relevant for several industries. For instance, laccase produced by *Trametes versicolor*, which is an extracellular enzyme integrated in the oxidoreductase group, can degrade a wide variety of organic and inorganic substrates. However, the downstream process of laccase from the fermentation broth remains a bottleneck, mostly due to the requirement of expensive equipment, low recovery and/or low activity of the resultant enzyme. Therefore, other approaches should be investigated to increase the purification and concentration of laccase, such as aqueous biphasic system (ABS). In this work, ABS composed of ionic liquids (ILs) or amino acids and polymers were investigated for the recovery of *T. versicolor* laccase from the fermentation broth. The studied ABS offered favorable purification conditions for laccase concentration.

[P-BB40]

Exploring glutathione as an adjuvant of anti-biofilm strategies against *Pseudomonas aeruginosa*

R. Monteiro, M.O. Pereira, A.M. Sousa*
Centre of Biological Engineering, LIBRO-Laboratório de Investigação em Biofilmes Rosário de Oliveira, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal
** anamargaridasousa@deb.uminho.pt*

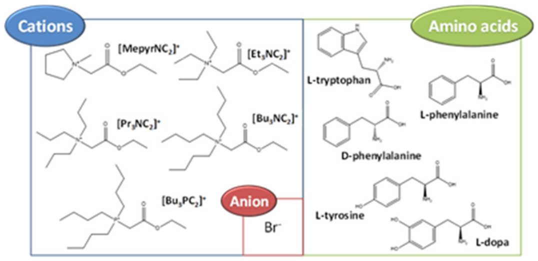


Pseudomonas aeruginosa biofilms are involved in several infectious diseases and their eradication remains a challenge. Disrupting the biofilm matrix is the most attractive way to facilitate biofilm-cells eradication and glutathione has been exhibiting great potential as a biofilm disrupter agent. Therefore, this study aimed to explore anti-biofilm strategies based on the combination of glutathione with two in-use antibiotics. Biofilms were formed and subjected to the action of combinatorial arrangements of glutathione with ciprofloxacin or tobramycin. Preliminary results showed that PAO1 biofilms were eradicated using glutathione+ciprofloxacin, in contrast to biofilms formed by a clinical isolate (PAI). Better outcomes were obtained using glutathione+tobramycin since biomass reduction occurred with lower dosages. Also, a different action than the usually described for glutathione is suggested. In conclusion, glutathione-tobramycin could be a potential anti-biofilm strategy.

[P-BB41]

Novel glycine betaine ionic liquids analogues as components of aqueous biphasic systems with improved performance to separate amino acids

A.F.C.S. Rufino[1], M.E. Rosa[1], M.M. Pereira[1], M.R. Almeida[1], J. Gomes[1], J.A. P. Coutinho[1], A. Mohamadou[2], M.G. Freire[1]*
[1]CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal; [2]Université de Reims Champagne-Ardenne, Institut de Chimie Moléculaire de Reims (ICMR), CNRS UMR 7312, UFR des Sciences Exactes et Naturelles, BP 1039, F-51687 Reims cedex 2, France.
**maragfreire@ua.pt*

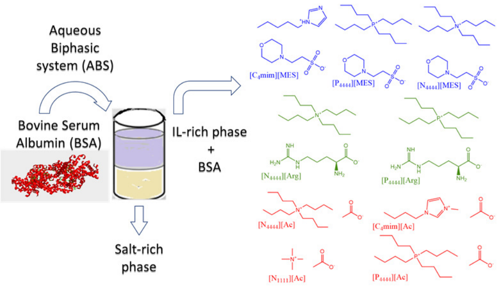


Given the biotechnology advances observed in recent years in terms of upstream, the development of effective downstream processes becomes mandatory to decrease the associated costs of biotechnological-based products. Although a large interest has been devoted to ionic-liquid-based aqueous biphasic systems (IL-based ABS) as tailored separation platforms, imidazolium-based ILs have been the preferred choice as phase-forming agents. To overcome some toxicity and biodegradability issues associated to imidazolium-based ILs, novel ABS composed of ILs analogues of glycine-betaine (AGB-ILs) are here proposed and investigated. The ABS phase diagrams were determined for mixtures composed of water, AGB-ILs and Na_2SO_4 at 298 K. Their performance as extraction strategies was evaluated with five amino acids. In all studied systems, amino acids preferentially migrate to the IL-rich phase, with amino acid one-step extraction efficiencies ranging between 65% and 100%.

[P-BB42]

Ionic-liquid-based aqueous biphasic systems as enhanced extraction platforms for bovine serum albumin

*A.F.C.S. Rufino, M.R. Almeida, M. Sharma, J.A.P. Coutinho ,M.G. Freire**
CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.
** maragfreire@ua.pt*

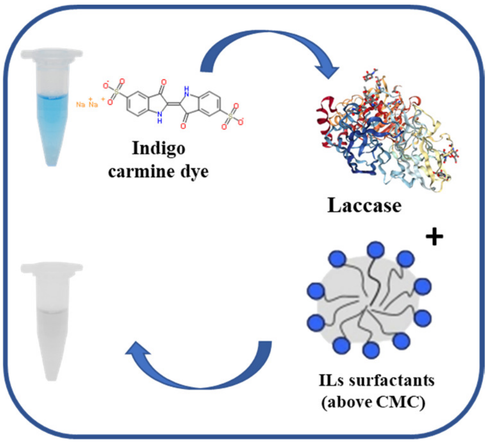


Aqueous biphasic systems (ABS) have been frequently applied in the extraction and purification of several biomolecules, such as proteins. In the last ten years, it has been demonstrated that ionic-liquid-based ABS (IL-ABS) allow remarkable extraction efficiencies and high selectivity in comparison with traditional polymer-based ABS. In this sense, a set of ILs was synthetized and characterized, and applied in the development of novel ABS formed with K_2HPO_4/KH_2PO_4 buffer at pH 7. The influence of the anion and the cation of the IL in the formation of ABS was evaluated by the determination of the respective liquid-liquid phase diagrams. Finally, their performance as extraction strategies was appraised with bovine serum albumin (BSA). In all the studied ABS, BSA preferentially migrates to the IL-rich phase, with extraction efficiencies of 100% achieved in a single-step.

[P-BB43]

Removal of dyes using surfactant ionic liquids for in situ biodegradation with laccase

R. Bento[1], M.C. Neves[1], J.A.P. Coutinho[1], A.M. P. Tavares[1], M.G. Freire[1]
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro, Portugal.
ruib@ua.pt

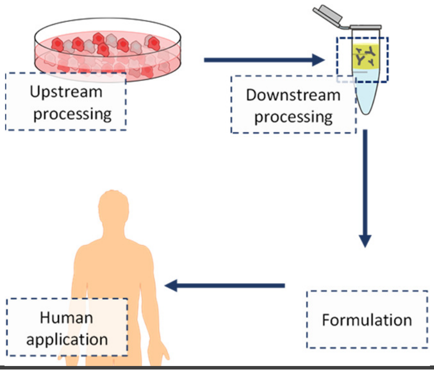


Increased contamination of water is a serious threat to human health and ecosystem. In this sense, effective approaches for the treatment of aqueous wastes, aiming at eliminating their detrimental effects and reduce costs, should be investigated. The use of surfactants that can incorporate enzymes for the degradation of pollutants can be considered as a potential alternative. Some enzymes are more active in micellar systems. In this work, biocompatible surfactant-based ILs were used to encapsulate colored pollutants and oxidative enzymes within the micelles for in situ biodegradation of persistent pollutants. Three dyes namely indigo carmine, remazol brilliant blue R and rhodamine 6G were used as models. At the optimized conditions, a high and fast dye degradation (>90%) was achieved for indigo carmine, by using surfactant-based ILs, namely, decyltrimethylammonium bromide. Micellar systems using surfactant IL is a promising methodology for the treatment to aqueous effluents treatment.

[P-BB44]

Development of an alternative bio-based process for the extraction and purification of monoclonal antibodies

*A.E. Santiago[1], E.V. Capela[1,2], A.P.M. Tavares[1], M.M. Pereira[1], A. Mohamadou[3], J.A.P. Coutinho[1], M.R. Aires-Barros[2], A.M. Azevedo[2], M.G. Freire[1]**
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal; [2] iBB - Institute for Bioengineering and Biosciences, Department of Bioengineering, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal; [3]ICMR – Institute of Molecular Chemistry of Reims, University of Reims Champagne-Ardenne, Reims, France.
**maragfreire@ua.pt*

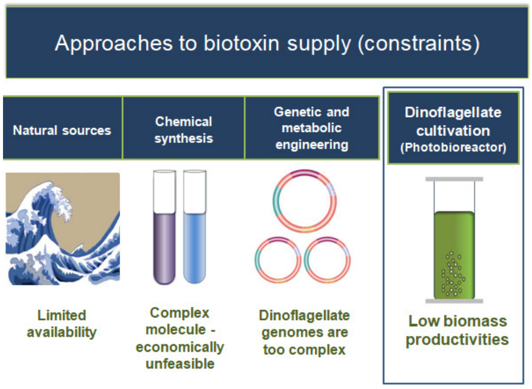


In this work, a more biocompatible and alternative platform was developed for the downstream processing of monoclonal antibodies, directly from Chinese Hamster Ovary (CHO) cell culture supernatants. This platform is based on the use of glycine-betaine analogous ionic liquids as phase-forming components of aqueous biphasic systems, which proved to greatly improve the extraction yield and the purification level of the target antibodies.

[P-BB45]

Dinoflagellates: unique microalgae for sustained supply of bioactive compounds

*J.L. Assunção[1, *] A.C. Guedes[2], F.X. Malcata[1, 3]*
[1] LEPABE – Laboratory of Process Engineering, Environment, Biotechnology and Energy, Rua Dr. Roberto Frias, s/n, P-4200-465, Porto, Portugal; [2] Interdisciplinary Centre of Marine and Environmental Research (CIIMAR), University of Porto,Terminal de Cruzeiros do Porto de Leixões, Avenida General Norton de Matos, s/n, P-4450-208, Matosinhos, Portugal; [3] Department of Chemical Engineering, University of Porto, Rua Dr. Roberto Frias, s/n, P-4200-465, Porto, Portugal.
** joanaleonardoassuncao@gmail.pt*

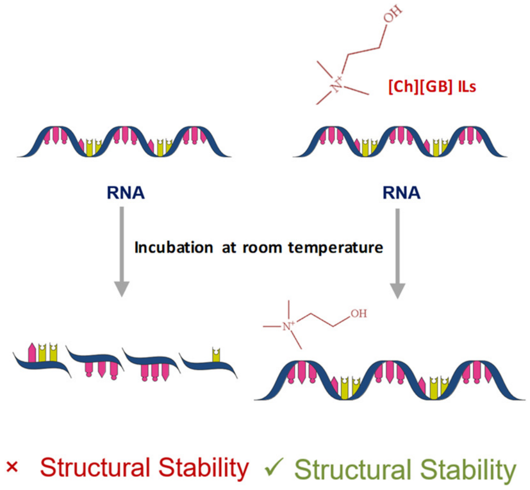


An interest in biotoxins produced by dinoflagellates has boomed in recent years. Such compounds exhibit a wide chemical diversity and complexity, and possess remarkable bioactivities – thus holding a strong potential for application as pharmaceutical leads. However, their production to sufficient extent remains an issue, thus hampering preclinical testing and eventual commercial exploitation. Such strategies as *de novo* chemical synthesis or genetic engineering are too laborious or even unfeasible at present. The most reasonable approach is dinoflagellate culturing in photobioreactor – yet unique designs and improved operating conditions are a must; their being fastidious microorganism and extremely sensitive to shear stress pose indeed serious challenges. Advances so far have encompassed culture medium formulation and light supply *in situ*; improvement of classical designs and proposal of novel configurations for dinoflagellate growth are under way.

[P-BB46]

Biological-based ionic liquids as novel preservation media for recombinant RNA

A. Q. Pedro[1,], P. Pereira[2,3], M. J. Quental[1], A. P. Carvalho[1], S. M. Santos[1], J. A. Queiroz[1], F. Sousa[3], M. G. Freire[1]*
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, Universidade de Aveiro, Portugal; [2] ITQB – Institute of Biologic and Chemical Technology, Universidade Nova de Lisboa, Oeiras, Portugal; [3] CICS-UBI – Health Sciences Research Centre, Universidade da Beira Interior, 6200-506 Covilhã, Portugal.
** apedro@ua.pt*

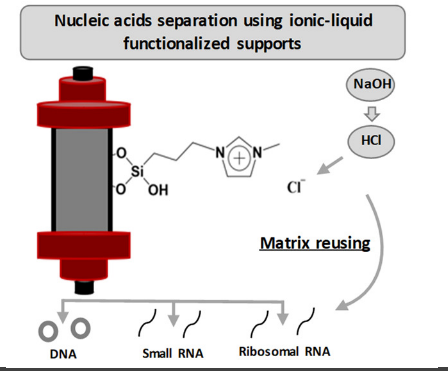


Nucleic-acid-based products have been identified as promising biopharmaceuticals and as relevant biomolecules in biological assays; however, the preservation of the RNA stability is still a remarkable challenge. Herein, we demonstrate the enhanced potential of aqueous solutions of self-buffering cholinium-based Good's buffers ionic liquids (GB-ILs) for extending the shelf life of a recombinant small RNA (sRNA) fraction derived from *Escherichia coli*, containing the therapeutically relevant microRNA. It was found that ILs comprising the cholinium (Ch) cation combined with anions derived from Good's buffers (MES, TES, HEPES, Tricine) are able to maintain the sRNA stability, at least up to 30 days, and thereby increase the RNA shelf life. In summary, aqueous solutions of [Ch][MES] and [Ch][HEPES] as remarkable stabilizing media of recombinant sRNAs at room temperature, without requiring the typically carried out samples freezing, thus reinforcing their effectiveness in RNA bioprocessing.

[P-BB47]

Separation of nucleic acids using ionic-liquid functionalized macroporous supports

P. Pereira[1,2], M.C. Neves[3], A.Q. Pedro[3,], I. Rodrigues[1], J.C. Martins[1], T. Trindade[3], J.A. Queiroz[1], M.G. Freire[3], F. Sousa[1]*
[1] CICS-UBI – Health Sciences Research Centre, Universidade da Beira Interior, 6200-506 Covilhã, Portugal; [2] ITQB – Institute of Biologic and Chemical Technology, Universidade Nova de Lisboa, Oeiras, Portugal; [3] CICECO – Aveiro Institute of Materials, Department of Chemistry, Universidade de Aveiro, Portugal.
**apedro@ua.pt*

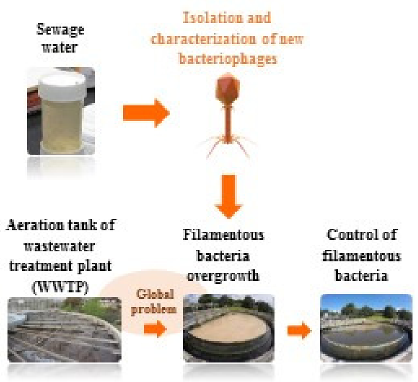


The preparation and characterization of novel macroporous chromatographic supports functionalized with ionic liquids, and with remarkable features in preparative liquid chromatography of nucleic acids, namely in selectivity, robustness and reproducibility, is here described. It is demonstrated that the ionic liquids act as multimodal ligands, while allowing the effective separation of nucleic acids, namely recombinant small RNAs, ribossomal RNAs, and genomic DNA obtained from a bacterial lysate. These supports can be easily regenerated and reused without compromising they performance.

[P-BB48]

Isolation and preliminary characterization of a new bacteriophage against *Sphaerotilus natans*

R. Ferreira[*], *R. Amado*[*], *J. Padrão, S. Santos, V. Ferreira, S. Cortez, J. Azeredo, M. Mota, A. Nicolau*
CEB – Centre of Biological Engineering, University of Minho, 4710-057 Braga, Portugal.
** protozoa@deb.uminho.pt*

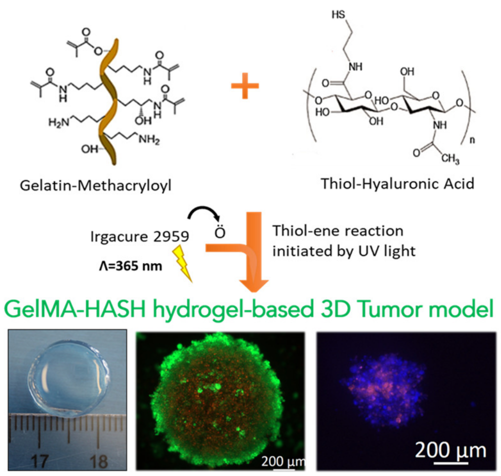


Activated sludge process, the most commonly used system for biological wastewater treatment, is driven by a community of microorganisms that play a key role in the conversion of the organic matter and removal of nutrients from wastewater. In this artificial ecosystem, filamentous and floc-forming bacteria co-exist in a dynamic equilibrium. However, filamentous bacteria overgrowth lead to a decrease of performance of the plant by causing two well-known phenomena: bulking and/or foaming. *Sphaerotilus natans* is a filamentous bacterium that can cause or contribute to the malfunction of these systems by leading to bulking occurrence. Bacteriophages are regarded as possible novel treatment against the filamentous overgrowth. In this work, the isolation and preliminary characterization of a new lytic bacteriophage against *S. natans* are described. Results clearly indicate the potential effect of this bacteriophage for future wastewater treatment system management.

[P-BB49]

Bioengineered *in vitro* 3D hydrogel-based cancer model using chemically modified biopolymers

M.V. Monteiro[1,*], *V.M. Gaspar*[1], *J.F. Mano*[1]
[1] *Department of Chemistry, CICECO – Aveiro Institute of Materials, University of Aveiro, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal.*
** m.monteiro@ua.pt*

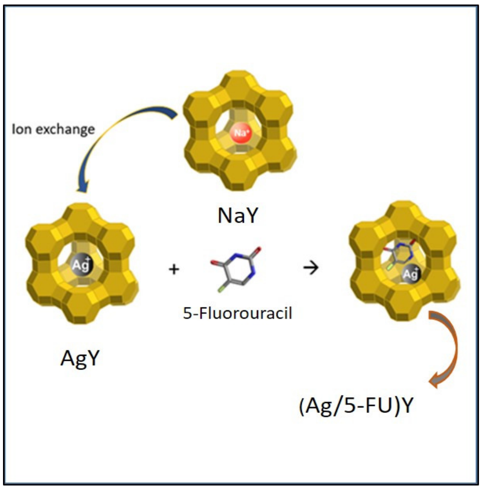


The development of hydrogel-based *in vitro* models using nature-derived bioactive materials such as gelatin and hyaluronic acid, is a promising approach for the discovery of new anti-tumor therapies in a faster and expeditious way. Herein we describe the chemical modification of gelatin and hyaluronic acid and subsequently engineering a photocrosslinking hydrogel composed of gelatin-methacryloyl and hyaluronic acid modified with thiol groups (GelMA-HASH), which intends to mimic the extracellular matrix of tumor microenvironment. *In vitro* multicellular 3D models, composed of cancer cells and fibroblasts, were also produced to mimic the cellular heterogeneity present in this disease. Each macromer was characterized by ^{1}H NMR and the biological functionality and viscoelastic properties of the 3D models produced by GelMA-HASH hydrogels were evaluated. Globally, the formulated hydrogel was considered to be a promising scaffold for bioengineering of 3D *in vitro* prostate cancer models and is envisioned to be used as a drug screening platform in the future.

[P-BB50]

Dual nanomaterial systems aiming antimicrobial activity and cancer treatment

P.R. Correia[1,2*], *C. Almeida-Aguiar*[2,3,4], *A.M. Fonseca*[1,3], *F. M. Baltazar*[5,6], *I.C. Neves*[1,3**]
[1] CQUM, Center of Chemistry, University of Minho, 4710-057 Braga, Portugal; [2] CITAB, Center for the Research and Technology of Agro-Environmental and Biological Sciences, University of Minho, 4710-057 Braga, Portugal; [3] CEB, Center of Biological Engineering, University of Minho, 4710-057 Braga, Portugal; [4]CBMA, Center of Molecular and Environmental Biology, University of Minho, 4710-057 Braga, Portugal; [5] Life and Health Sciences Research Institute (ICVS), School of Medicine, University of Minho, 4710-057 Braga, Portugal; [6]ICVS/3B's - PT Government Associate Laboratory, Braga/Guimarães, Portugal.
**pg31433@alunos.uminho.pt ; **ineves@quimica.uminho.pt*

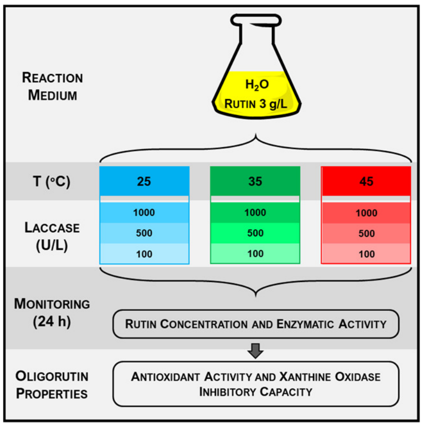


In the 21st century, nanotechnology has been emerging as a very promising field, with numerous applications in distinct areas, such as textiles, food agriculture, environment, electronics and in the biomedical field. Among the different categories of nanomaterials, zeolites are a very important class of inorganic materials that have been used in a wide range of applications. In the current work, we used zeolite NaY as host to incorporate silver ions and the antineoplastic drug 5-Fluorouracil (5-FU) for microbial infections and non-melanoma skin cancer treatment, respectively. Both situations present a major threat to public health: microbial infections due to their increasing resistance to antibiotics and cancer because of the difficulty of an efficient treatment especially when the disease has progressed considerably. So, since zeolites have a range of structural and physical properties that make them suitable for therapeutic delivery systems, they could be interesting candidates for this purpose. Our goal is to create an efficient and biocompatible dual topical delivery system with zeolites and, this way, combine the antimicrobial and the antineoplastic activity in the same formulation.

[P-BB51]

Effect of temperature and laccase activity on the production of oligorutin in a reaction medium free of organic solvents

A. Muñiz-Mouro[*], *B. Gullón, T. A. Lú-Chau, M. T. Moreira, J. M. Lema, G. Eibes*
Department of Chemical Engineering, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain
**abel.muniz@usc.es*

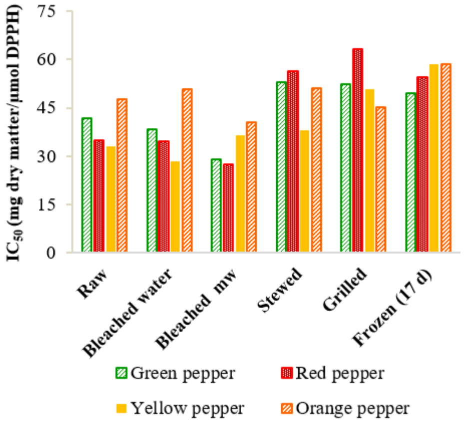


The enzymatic polymerization of rutin has been proved as an efficient method for obtaining products with enhanced properties, but in most cases, toxic solvents are needed to increase the initial substrate concentration. In this work, the possibility of producing rutin oligomers starting at a concentration beyond rutin aqueous solubility in a reaction medium without co-solvents was studied paying attention to the effect of the initial laccase activity used (1000-500-100 U/L) and the temperature at which reactions took place (25-35-45ºC). Results obtained shown that the reaction did not affect the xanthine oxidase inhibitory activity, but it reduced the antioxidant activity, with this decrease being comparable for products obtained using 1000 and 500 U/L, for all temperatures. It was also possible to conclude that shortening the reaction time down to 6 h would lead to a reasonable high rutin conversion with no apparent loss in enzymatic activity when starting the reaction with 1000 U/L.

[P-BB52]

Effect of processing on the antioxidant activity of different varieties of peppers (*Capsicum annuum*)

N. Alua[1,2], *<u>M. C. Serra</u>*[1,2*]
[1]*Área Departamental de Engenharia Química, ISEL, Lisboa, Portugal*
[2]*Centro de Estudos de Engenharia Química, ISEL, Lisboa, Portugal*
** mcserra@deq.isel.ipl.pt*



Vegetables have bioactive components (polyphenols, phytosterols, carotenoids, glucosinolates) that lead to important health benefits. However, there are vegetables that to be preserved or ingested, need to undergo heat treatments which can cause changes in physicochemical properties, composition and antioxidant activity [1,2].

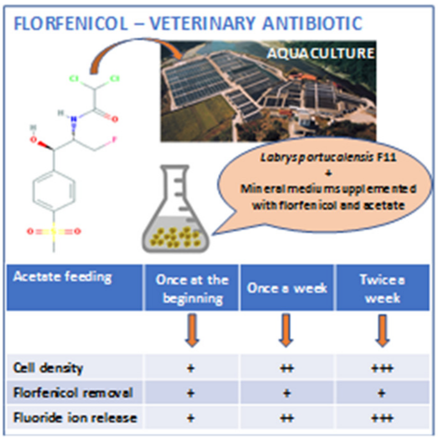
In this work, the antioxidant activity of different types of peppers (green, red, yellow and orange), raw and submitted to processing (hot water and microwave bleaching, stewed, grilling and frozen) was evaluated and expressed in IC_{50}. After extraction with a solution of ethanol-water 80 %, the extracts were analyzed for its ability to inhibit radicals of 2,2-diphenyl-1-picrylhydrazyl (DPPH).

The antioxidant activity of the extracts depends on the peppers variety with IC_{50} values from 32.8±3.6 to 47.7±2.7 mg dry matter/µmol DPPH in raw yellow and orange peppers, respectively. Regarding the type of processing, some variations in these IC_{50} results were found.

[P-BB53]

Bacterial degradation of the veterinary antibiotic florfenicol

<u>A.T. Couto</u>[1, *], *C.L. Amorim*[1,2], *P.M.L. Castro*
[1]*Universidade Católica Portuguesa, CBQF - Centro de Biotecnologia e Química Fina – Laboratório Associado, Escola Superior de Biotecnologia, Rua Arquiteto Lobão Vital, 172, 4200-374 Porto, Portugal;* [2]*Biology Department and CESAM, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*
**atcouto@porto.ucp.pt*



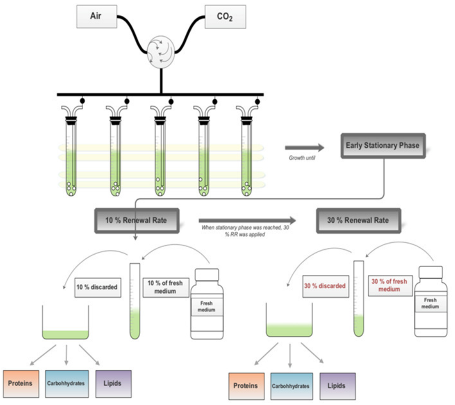
Acetate feeding	Once at the beginning	Once a week	Twice a week
Cell density	+	++	+++
Florfenicol removal	+	+	+
Fluoride ion release	+	++	+++

Florfenicol (FF) is an antibiotic largely used in aquaculture and its presence in their aqueous streams can affect the treatment process. Bacteria can play an important role in the cleanup of contaminated sites due to their ability to degrade an impressive variety of pollutants, using them as carbon and energy source. This study aimed to investigate the degradation of FF by a single bacterial strain, *Labrys portucalensis* F11. Biodegradation of FF was assessed in batch mode in the presence of a conventional carbon source and the bacterium was capable to remove ca. 80% of the FF supplied. When acetate was periodically added, although the cell growth was improved, no effect on the uptake of FF was observed but its defluorination was greatly enhanced.

[P-BB54]

Changes in the biochemical composition of selected *Tetraselmis* species, cultured semi-continuously under distinct renewal rates

V. Pôjo[1, *], *A. Otero*[2], *F.X. Malcata*[1]
[1] LEPABE, Department of Chemical Engineering, University of Porto, R. Dr. Roberto Frias, 4200-465, Porto, Portugal; [2] Instituto de Acuicultura, Campus Vida, Universidade de Santiago de Compostela, 15782, Santiago de Compostela, Spain.
* vpojo@fe.up.pt

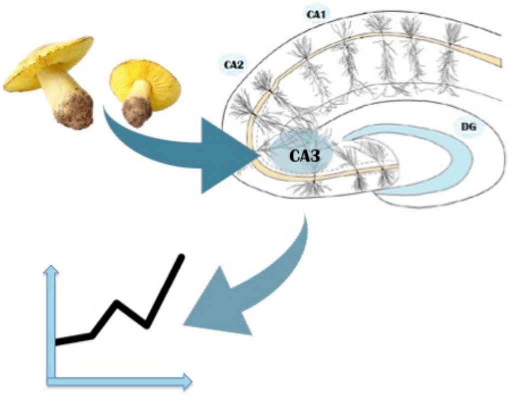


Several strains of *Tetraselmis suecica* (UW 605 and AROSA) and of *Tetraselmis sp.* that were characterized as lipogenic (RG 63, RG 75 and RG 74) and non-lipogenic (RG 44 and RG 46) through the flotation method were cultured semi-continuously using two different daily renewal rates, 10 % and 30 % of the volume of the cultures, in attempts to ascertain the changes in production rates of proteins, carbohydrates and lipids. As expected, an increase in renewal rate produced an increase in protein content of the biomass but a decrease in carbohydrate content in all strains. Lipid content decreased for RG 63 and RG 74 strains (lipogenic) with a renewal rate of 30 % and increased for RG 44 and RG 46 strains (non-lipogenic). Our results prove the influence of cultivation mode upon the biochemical composition of microalgae.

[P-BB55]

Effect of polysaccharides in neuronal ROS production

C. Miranda[1], *M. Batista*[1], *M. Bosio*[1,2,3], *A. Pessoa*[1], *E. Saggioro*[3], *M. Dezotti*[2], *J. Bassin*[2], *G. Marques*[4], *F. Nunes*[5], *R.M. Quinta-Ferreira*[1], *M.E. Quinta-Ferreira*[,6*]
[1]*CIEPQPF – Chemical Engineering Processes and Forest Products Research Center Department of Chemical Engineering, University of Coimbra, Rua Sílvio Lima, Coimbra – 3030-790, Portugal ;* [2]*Programa de Engenharia Química - PEQ/COPPE, Universidade Federal do Rio de Janeiro, P.O. Box 68502, 21941-972, Rio de Janeiro, RJ, Brazil;* [3]*Sanitation and Environment Health Department, Sergio Arouca National School of Public Health, Oswaldo Cruz Foundation, Avenida Leopoldo Bulhões, 1480, Rio de Janeiro – 21041-210, Brazil;* [4]*CITAB – Centre for the Research and Technology of Agro-Environment and Biological Sciences, Department of Agronomy, University of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal,* [5]*CQ - Chemistry Research Centre, Chemistry Department, University of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal.* [6]*Center for Neurosciences and Cell Biology and Physics Department, University of Coimbra, Rua Larga, Coimbra – 3004-516, Portugal.*
** emilia@uc.pt*



With the increasing number of diseases caused by harmful daily actions there is a greater demand for natural products with antioxidant properties. Antioxidants have a very important role in reducing the oxidative damage caused by free radicals, such as reactive oxygen species (ROS). This type of cellular damage is involved in many diseases such as cancers, neural disorders and premature aging. The aim of this study was to evaluate the effect of polysaccharides extracted from the mushroom *Tricholoma equestre*, in the formation of neuronal ROS, using the fluorescent indicator H2DCFDA. The experiments were performed in brain slices, using a polysaccharide mixture at the concentrations of 0.1 $g.L^{-1}$, 0.5 $g.L^{-1}$ and 1 $g.L^{-1}$. Significant changes were observed only for the 1 $g.L^{-1}$ concentration, which indicated a decrease of about 5 % in ROS production. The observed inhibition is in agreement with the idea that the used polysaccharides have an antioxidant action.

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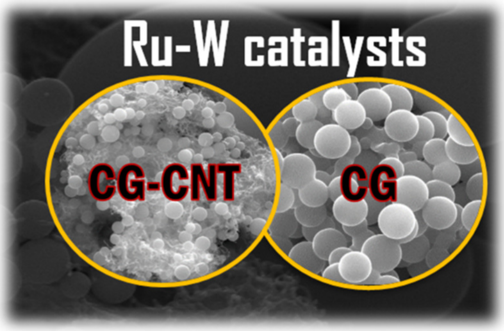
Poster Session

BIOREFINERY AND SUSTAINABILITY

[P-BS01]

Direct transformation of cellulose to ethylene glycol using Ru-W bimetallic catalysts supported on glucose-derived carbon materials

L.S. Ribeiro[1,*], *N. Rey-Raap*[1], *J.L. Figueiredo*[1], *J.J.M. Órfão*[1], *M.F.R. Pereira*[1]
[1] *Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.*
* *lucilia@fe.up.pt*

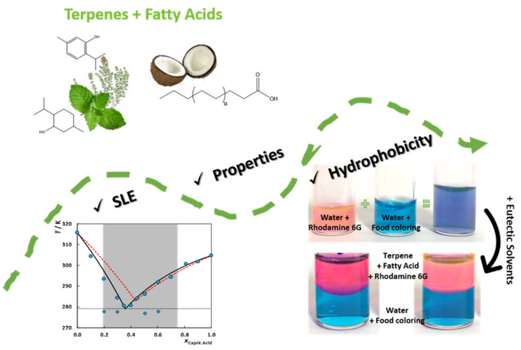


The catalytic conversion of lignocellulosic biomass to valuable chemicals has attracted global interest. In this work, Ru-W bimetallic catalysts supported on glucose-based carbon materials were synthesized to perform the hydrolytic hydrogenation of cellulose to ethylene glycol (EG) in a single step. The catalysts were examined for the one-pot reaction and have shown to be efficient for the direct production of EG from cellulose. Conversions of cellulose of 100 % were achieved in just 2 h of reaction and yields of ethylene glycol up to 35 % were obtained after 5 h. The prepared materials are promising alternatives to carbon nanotubes and other materials as catalyst supports for the production of EG directly from cellulose in a more economic, sustainable, faster and easier way.

[P-BS02]

Tunable hydrophobic eutectic solvents based on terpenes and monocarboxylic acids

M.A.R. Martins[1-4,*], *E.A. Crespo*[1,5], *P.V.A. Pontes*[4], *L.P. Silva*[1], *M. Bülow*[5], *G.J. Maximo*[4], *E.A.C. Batista*[4], *C. Held*[5], *S.P. Pinho*[2,3], *J.A.P. Coutinho*[1,*]
[1] *CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal;* [2] *Associate Laboratory LSRE-LCM, IPB, 5300-253 Bragança, Portugal;* [3] *Mountain Research Center – CIMO, IPB, 5301-855 Bragança, Portugal;* [4] *Faculty of Food Engineering, University of Campinas, 13083-862 Campinas, Brazil;* [5] *Laboratory of Thermodynamics, TU Dortmund, 44227 Dortmund, Germany;*
* *moniamartins@ua.pt ; jcoutinho@ua.pt*

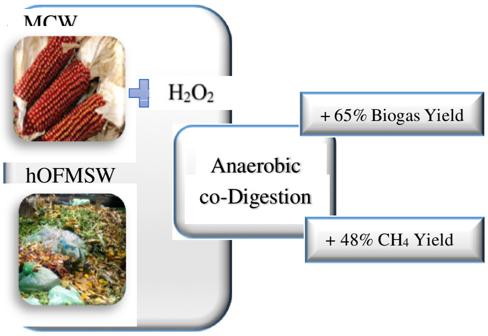


Recently some works claim that hydrophobic deep eutectic solvents could be prepared based on menthol and monocarboxylic acids. Despite of some promising potential applications these systems were poorly understood and this work addresses this issue. Here the characterization of eutectic solvents composed by the terpenes thymol or L(–)-menthol and monocarboxylic acids is studied aiming the design of these solvents. Their SLE phase diagrams were measured by differential scanning calorimetry in the whole composition range, showing that a broader composition range, and not only fixed stoichiometric proportions can be used as solvents at low temperatures. Moreover, the densities, viscosities, solvatochromic parameters and mutual solubilities with water were measured at compositions close to the eutectic point. The mutual solubilities with water attest the hydrophobic character of the mixtures investigated. The experimental SLE phase diagrams were described using the PC-SAFT EoS.

[P-BS03]

Pre-treatment of maize cob waste with hydrogen peroxide for biogas enhancement

E. Surra[1], M. Bernardo[2], N. Lapa[1], I.A.A.C. Esteves[2], I. Fonseca[2], J.P.B. Mota[2]*
[1] LAQV-REQUIMTE, Departamento de Ciências e Tecnologia da Biomassa, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal; [2] LAQV-REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal.
** ncsn@fct.unl.pt*

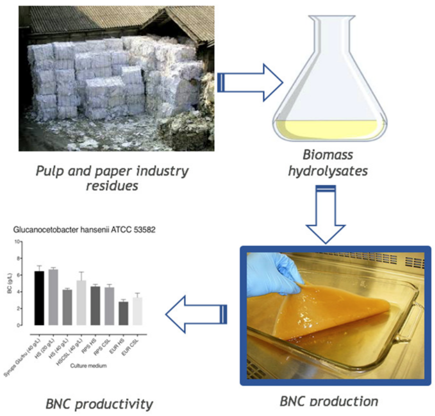


The enhancement of biogas and CH_4 yields through anaerobic co-digestion (co-AD) of the pre-hydrolysed Organic Fraction of Municipal Solid Waste (hOFMSW) and Maize Cob Waste (MCW) was tested in a lab-scale thermophilic anaerobic reactor. This enhancement is relevant if the biogas has to be upgraded to biomethane. Before the co-AD, MCW was chemically pre-treated with H_2O_2 at room temperature and optimized conditions of MCW percentage and reaction time. The co-AD of hOFMSW with MCW, pre-treated with 10% MCW $w_{MCW}/v_{alkaline\ water}$ for 4h of contact time and a w_{H2O2}/w_{MCW} ratio of 0.5, increased the biogas and CH_4 production yields by 65% and 48%, respectively, when compared to the results obtained with the standalone hOFMSW. Moreover, during this co-AD assay, the biogas stream provided a Low Heating Value (LHV) and a daily biogas energy content of 4 % and 1 % higher, respectively, than those obtained with co-AD of hOFMSW with non-pre-treated MCW.

[P-BS04]

Bacterial cellulose production through hydrolysates produced with cellulosic residues

F. Garrett, A. Rodrigues, F. Dourado, M. Gama[3]*
[1]CEB - Centro de Engenharia Biológica, departamento de engenharia biológica, Universidade do Minho, Gualtar, Braga, Portugal.
** francisco.agss@gmail.com*



In the paper industry, significant fraction of fibers that cannot be re-utilized are wasted by the paper companies, which raise economic and environmental concerns. An increasing demand of bacterial cellulose (BC) has been noticed in the last years. In order to ally the recycling of lignocellulosic residues and the production of bacterial cellulose, Recycled paper sludge (RPS) and rejected fibers (EUR) were enzymatically hydrolyzed to obtain sugar hydrolysates, which were used for BC production. Exploratory assay (different strains and nitrogen sources) was performed with RPS and EUR hydrolysates. RPS hydrolysate showed to be an interesting an alternative carbon source for *G. hansenii* (5 g/L of BC) and EUR hydrolysate showed potential as carbon source for *G. xylinum* (4-5 g/L of BC). Overall, the results suggest that RPS and EUR residues have potential to be alternatives of carbon source for BC production, after a further optimization of the BC production and the enzymatic hydrolysis.

[P-BS05]

Assessment of agroforestry residues potential within the biorefinery context

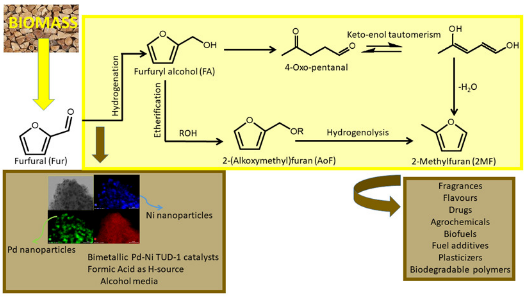
M. C. Gaspar; C. Mendes; S. R. Pinela; R. Moreira; M. G. Carvalho; M .J. Quina; M. E. M. Braga; A. T. Portugal**
CIEPQPF, Chemical Process Engineering and Forest Products Research Centre. Department of Chemical Engineering, University of Coimbra, Portugal.
**atp@eq.uc.pt ; marabraga@eq.uc.pt*

The interest in converting biomass resources into energy and value-added bioproducts is increasing in modern societies. In this way, the aim of this work is to evaluate the potential of four Portuguese agroforestry residues within the biorefinery context: pine branches and stumps, winery and tomato industrial wastes. Volatiles and other extractable fractions with biological properties, such as repellent/attractant, antioxidant activity and flavonoid content were obtained, being these properties relevant for food, pharmaceutical, and agroforestry industries. The potential for biogas production was assessed and encouraging results were obtained. Stumps potential for bioethanol production was evaluated by their characterization in terms of holocellulose (cellulose and hemicellulose) content, while the potential for bio-oil production was estimated by solvolysis process. All residues are promising for a bio-based economy.

[P-BS06]

One-pot conversion of furfural to bioproducts over mesoporous bimetallic catalysts

M.M. Antunes[1,], S. Lima[2], A. Fernandes[3], M.F. Ribeiro[3], D. Chadwick[2], K. Hellgardt[2], M. Pillinger[1], A.A. Valente[1]*
[1] Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal; [2] Department of Chemical Engineering, Imperial College London, South Kensington Campus, London, SW7 2AZ, UK, [3] Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001, Lisbon, Portugal.
** margarida.antunes@ua.pt*



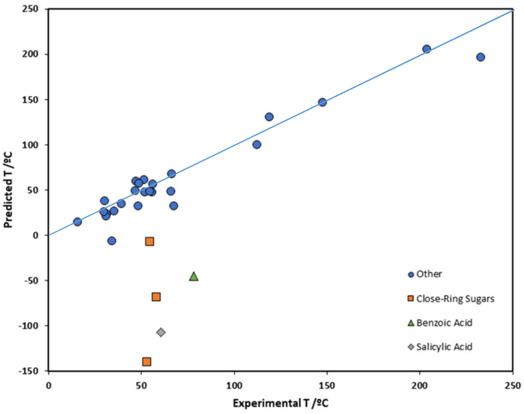
Scheme 1- Furfural conversion to useful bioproducts, namely 2-(alkoxymethyl)furan, 2-methylfuran, 4-oxopentanal and its acetals, via acid and reduction reactions, over a heterogeneous bimetallic catalyst.

The renewable platform chemical furfural is produced industrially, and used as solvent or intermediate for synthesizing various bioproducts with different applications in the chemical industry. The present work focusses on the production of the bioproducts 2-(alkoxymethyl)furans, 2-methylfuran, 4-oxopentanal and its acetals in one-pot from Fur. For such an achievement, bimetallic Pd-NiTUD-1 mesoporous catalysts were used. These multifunctional catalysts allowed the in situ hydrogen supply from formic acid, responsible for the reduction steps involved. Different procedures were applied for the synthesis of the materials, and the influence of the materials' properties on the catalytic performances was studied. Detailed characterization and catalytic studies (with the identification of reaction intermediates) led to insights into the reaction mechanism, the roles of the different types of metal species on the complex reaction mechanism, and the catalyst stability.

[P-BS07]

Using COSMO-RS to design choline chloride-based eutectic solvents

D.O. Abranches[1], M. Larriba[2], L.P. Silva[1], M. Melle-Franco[1], J.F. Palomar[3], S.P. Pinho[4,5], J.A. P. Coutinho[1,*]
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;
[2] Department of Chemical Engineering, Faculty of Chemical Sciences, Complutense University of Madrid, 28040, Madrid, Spain;
[3] Sección de Ingeniería Química, Universidad Autónoma de Madrid, Madrid 28049, Spain; [4] Associate Laboratory LSRE-LCM, Department of Chemical and Biological Technology, Polytechnic Institute of Bragança, Portugal; [5] Mountain Research Center – CIMO, Polytechnic Institute of Bragança, Portugal.
* jcoutinho@ua.pt



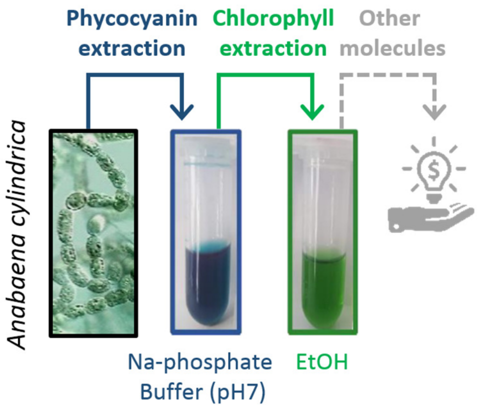
Deep eutectic solvents (DES) present interesting properties, mostly connected to their solvation ability, and have been subject to much research in the recent past. Currently, the discovery of new eutectic solvents is accomplished by experimentally measuring the eutectic point of random systems, often using choline chloride as a hydrogen bond acceptor.

In this work, new choline chloride-based eutectic systems were experimentally assessed. Their eutectic data, along with other previously reported in the literature, was used to evaluate a method based on COSMO-RS to predict the eutectic temperature of choline-chloride based mixtures. The predictive methodology herein developed allows for the quick scanning of a large matrix of systems in order to identify those more promising to be liquid at any given temperature. To validate the method here proposed, the eutectic temperature of pharmaceutical drug-based mixtures was predicted and, then, assessed experimentally, being shown that the COSMO-RS can be used to help design liquid drug-based formulations.

[P-BS08]

Sequential extraction of phycocyanin and chlorophyll from *Anabaena cylindrica*

T.E. Sintra[1,*], M. Martins[1], I.P.E. Macário[2], S.S. Bagagem[1], J.L. Pereira[2], F. Gonçalves[2], J.A.P. Coutinho[1], S.P.M. Ventura[1]
[1]CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193, Aveiro, Portugal [2]CESAM – Centre for Environmental and Marine Studies, Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal
*tania.sintra@ua.pt

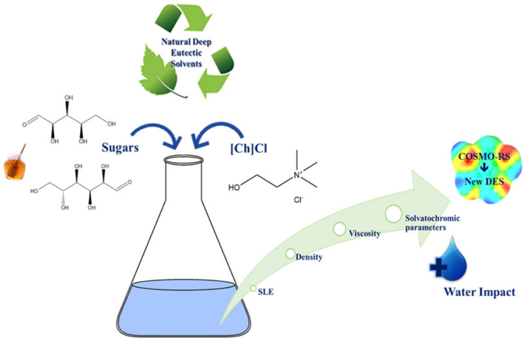


Cyanobacteria are attracting the attention worldwide as a reliable and sustainable feedstock for the production of biofuels, food colorants and biochemically active compounds. *Anabaena cylindrica* is a cyanobacterium with a significantly widespread occurrence in Portuguese freshwater habitats, with phycocyanin and chlorophyll in abundance. These compounds have a huge market value, namely phycocyanin with an expected market around $60 million by 2019. The present work focuses on the development of a sequential extraction methodology to obtain phycocyanin and chlorophyll from fresh samples of *Anabaena cylindrica*. Extracting several compounds from the same sample constitutes a great opportunity since they can later be applied in industry at lower costs and regarding less waste of biomass. The proposed process consists on a more sustainable method allowing the extraction of around 90% and 55% of phycocyanin and chlorophyll, present in the sample, respectively.

[P-BS09]

Analyzing sugar-based NADES: A study based on experimental measurements of solid-liquid phase diagrams and their modeling using COSMO-RS

L.P. Silva,[1] *L. Fernandez,*[2] *J. Conceição,*[1] *M.A.R. Martins,*[1,3,4] *A. Sosa,*[2] *J. Ortega,*[2] *S.P. Pinho,*[3,4] *J.A.P. Coutinho*[1]
[1]CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;[2]Laboratorio de Termodinamica y Fisicoquímica de Fluidos, Universidad de Las Palmas de Gran Canaria, 35071 – Parque Científico-Tecnológico, Canary Islands, Spain; [3]Associate Laboratory LSRE-LCM, Department of Chemical and Biological Technology, Polytechnic Institute of Bragança, 5300-253 Bragança, Portugal;[4]Mountain Research Center – CIMO, Polytechnic Institute of Bragança, 5301-855 Bragança, Portugal.
**lilianapatrocinio@ua.pt*

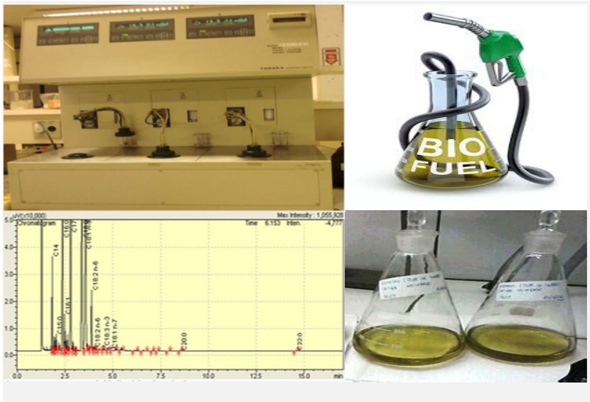


Natural based-DES are described as "green solvents" due to their low-toxicity, non-flammability, water-compatibility and negligible vapor pressure. Given the recent interest for NADES and the number of articles reporting applications using sugars as DES precursors, data on the solid-liquid equilibria(SLE) of their mixtures is surprisingly scarce, as well as their physical properties, despite the information it provides on the range of compositions and temperatures to operate these systems. In this work, we studied the SLE of binary and ternary mixtures involving [Ch]Cl+sugars.The experimental phase diagrams were described by two excess Gibbs energy(g^E) models, namely NRTL and a modified Redlich-Kister expansion, after used to develop tools for predicting the behavior of other sugar-based DES. Densities, viscosities, solvatochromic parameters and water impact were evaluated at the eutectic composition, in order to address the tailoring of their properties using water.

[P-BS10]

Experimental measurement and thermodynamic modeling of flow parameters sebum biodiesel cold

C.P.G. Lira[1*], *I.R.S. Araujo*[2], *A.E.X. Stragevitch*[3]
[1,2,3] *Laboratory of fuels- Federal University of Pernambuco, Recife, Brazil.*
[*] *cinthyapetrucia@hotmail.com*

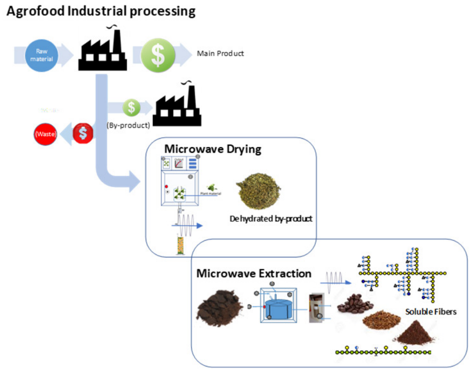


The work consists of experimental analyzes and computer simulations in animal fat derived biodiesel industry in which was used antifreeze additive VISCOPLEX, donated by Evonik Industries, S50 diesel donated by Suape Distributor BR and also commercial soybean oil to try to improve the cold flow properties of biodiesel studied. A portion of this work was the realization of physicochemical analyzes on biodiesel from animal fat to study the formation of a precipitate of unknown nature formed at low temperatures. The other portion was to determine the cloud point by computer simulation and compared with the experimentally obtained. To perform the computational model using chromatographic analyzes to determine the mass composition of biodiesel studied was required as well as the properties of thermophysical esters of saturated and unsaturated fatty acids, in particular about the melting enthalpy and melt temperature.

[P-BS11]

Microwave drying and/or extraction of bioactive compounds from industrial by-products

C. P. Passos[1,*], *S.S. Ferreira*[1], *S. Cardoso*[1], *D.F. Wessel*[2], *G.R. Lopes*[1], *A. Rudnitskaya*[3], *D.V. Evtuguin*[4], *M.A.Coimbra*[1]
[1]QOPNA, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal; [2]CI&DETS, Polytechnic Institute of Viseu – Agrarian Higher School, Quinta da Alagoa, Estrada de Nelas 3500-606, Viseu, Portugal; [3]CESAM, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal; [4]CICECO, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal
** cpassos@ua.pt*



Current circular economy concern has led industries to search for approaches able to reduce waste while increasing value of by-products. However, due to the typically high moisture content of the later, application of dehydration processes is almost mandatory [1]. The microwave technology can be used to dehydrate broccoli by-products while preserving a polysaccharide-rich residual product. This technology, based on hydrodiffusion and gravity, also allows for the simultaneous recovery of diffused water which, in the case of broccoli, contain up to 356 µg/mL glucosinolates [2].

[P-BS12]

IProPBio - Integrated Process and Product Design for Sustainable Biorefineries

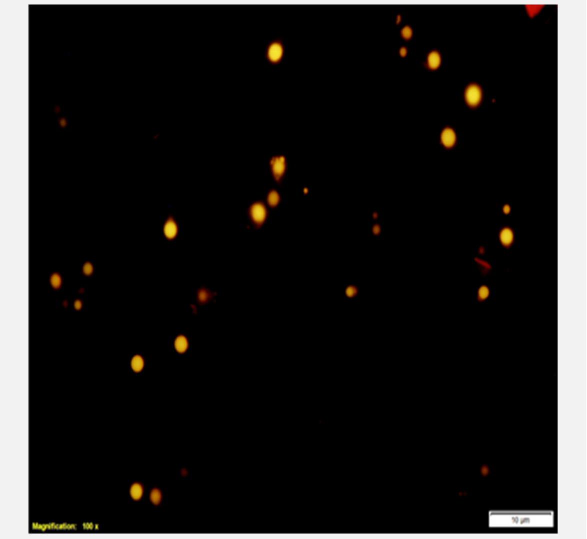
M. Errico[1,*], *J.P. Coelho*[2, 3],*M.P. Robalo*[2, 3] , *R.M. Filipe*[2, 4], *M. Martin*[5], *P. Angeli*[6], *R.P. Stateva*[7], *M. Papadaki*[8], *C. Pastore*[9], *S. Santzouk*[10],*H. Matos*[4, 11],*A. Bonilla-Petriciolet*[12], *M.El Halwagi*[13], *M.L. Corazza*[14]
[1]University of Southern Denmark, Department of Chemical Engineering, Biotechnology and Environmental Technology, 5230 Odense M, Denmark; [2] Department of Chemical Engineering, Instituto Superior de Engenharia de Lisbon (ISEL); [3]Centro de Quimica Estrutural, Instituto Superior Técnico (IST), University of Lisbon, Lisbon, Portugal; [4] CERENA, Instituto Superior Técnico, University of Lisbon, Lisbon, Portugal; [5]Department of Chemical Engineering, University of Salamanca, 37008 Salamanca, Spain; [6]11ThAMeS Multiphase, Department of Chemical Engineering, UCL, London WC1E 7JE, UK; [7]Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, Bulgaria; [8]Department of Environmental & Natural Resources Management, School of Engineering, Agrinio, GR30100, University of Patras, Greece; [9]Consiglio Nazionale delle Ricerche (CNR), Instituto Di Ricerca Sulle Acque(IRSA), 70132, Bari, Italy; [10]Santzouk Samir and Co. General Partnership, PANAX, Agios Konstantinos, Aetoloacarnania -Agrinio, GR30100, Greece;[11]Department of Chemical Engineering, Instituto Superior Técnico (IST); University of Lisbon, Lisbon, Portugal; [12]Instituto Tecnologico de Aguascalientes, Aguascalientes 20256, Mexico; [13]The Artie McFerrin Department of Chemical Engineering, TEES, Texas A&M University, Texas 77843-3122; USA; [14]Department of Chemical Engineering, Federal University of Paraná (UFPR), Paraná 81531-980, Brazil
*iprobio@kbm.sdu.dk

Bio-based economy involves in Europe 22 million people and turns over roughly 2.4 billion €. The full realization of its huge potential, however, requires expert knowledge and synergy of different competencies. The overall goal of IProPBio is to exchange complementary theoretical and experimental knowledge of research staff while looking for innovative answers in the field.IProPBio addresses key engineering, thermodynamic, energy, environmental, safety, production and process challenges in the design, optimization and operation of sustainable biorefinery. IProPBio will significantly impact: a) the competitiveness of EU bioeconomy; b) participants' potential and new carrier perspectives; c) exchange and transfer of high-quality multidisciplinary knowledge, advanced expertise, research and innovation between academic and non-academic participants in EU member states and third countries through the dissemination of the results achieved to target groups and the general public.

[P-BS13]

Simultaneous degradation of hydrocarbons and production of valuable compounds by *Yarrowia lipolytica*

M. Lopes[1,*], *R. Ramôa*[1], *S.M. Miranda*[1], *I. Belo*[1]
[1] *Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710-057 Braga, Portugal;*
**marlenelopes@deb.uminho.pt.*

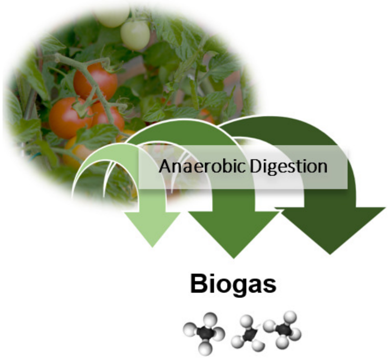


Hydrocarbons are dangerous pollutants and great amounts of these compounds are released to the environment, due to the inadequate handling in the petroleum extraction or in the effluents of industries that use petroleum or its derivatives. The ability of *Yarrowia lipolytica* to efficiently degrade hydrocarbons (herein demonstrated with hexadecane and hexadecene) and use them as carbon source to grow and produce valuable compounds was demonstrated. In hexadecane-based medium, *Y. lipolytica* W29 cells were able to accumulate up to 16 % of their cellular dry weight as intracellular lipids. Due to its composition, similar to that of vegetable oils, these microbial lipids can be used as feedstock for biodiesel production. Moreover, the simultaneous production of lipase (2730 $U \cdot L^{-1}$), which market demand is increasing due to its application in the field of bioenergy, represents an economic advantage. Thus, it is possible to valorize wastes contaminated with hydrocarbons with this bioprocess.

[P-BS14]

Valorisation of tomato wastes for energy production through anaerobic digestion

S.R. Pinela, R.P. Rodrigues. M.J. Quina[*]
[1]*CIEPQPF – Chemical Process Engineering and Forest Products Research Centre, Department of Chemical Engineering, University of Coimbra, Rua Sílvio Lima, 3030-790 Coimbra, Portugal.*
** guida@eq.uc.pt*

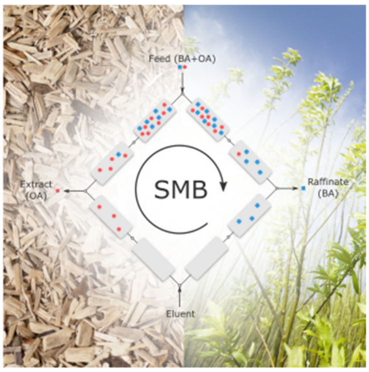


Toward a circular economy, there is an increasing interest in valorisation of agroindustry wastes. As a case study can be considered the tomato industry, which at the end of the campaign produces considerable quantities of wastes. This work aims to evaluate of three types of wastes: rotten tomato waste (TWR), green tomato waste (TWG) and branches of tomato waste (TWB) for biogas production through anaerobic digestion. The physical and chemical properties of these residues, such as pH, total and volatile solids, chemical oxygen demand, and elemental content were evaluated. Biochemical methane potential (BMP) was evaluated through both experimental and theoretical approaches. Results showed that the wastes analysed have potential for methane production, mainly TWR.

[P-BS15]

Separation of betulinic and oleanolic acids by simulated moving bed

I. S. Azenha[1], J. P. S. Aniceto[1], S. Sequeira[1], C. Areia[1] A. Mendes[2], C. M. Silva[1]*
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193, Aveiro, Portugal;
[2] LEPABE-Faculdade de Engenharia, Universidade do Porto, 4200-465 Porto, Portugal;
** carlos.manuel@ua.pt*



In this work, a simulated moving bed unit was designed for the separation of betulinic and oleanolic acids. HPLC pulse experiments were conducted to select suitable stationary and mobile phases, and best results were found with an Apollo C18 column with 50/50 (%, v/v) acetonitrile/methanol mixture. Breakthrough experiments of pure components were conducted to determine equilibrium and mass transport parameters. They were then successfully validated through the simulation of a breakthrough assay of a binary mixture of these acids. Rigorous phenomenological simulation results showed that the SMB unit successfully separates the compounds with purities above 99 % (wt. %) from a representative natural extract of *Eucalyptus globulus* bark containing the triterpenic acids under study.

[P-BS16]

Sustainable microalgae biorefinery development through process optimization

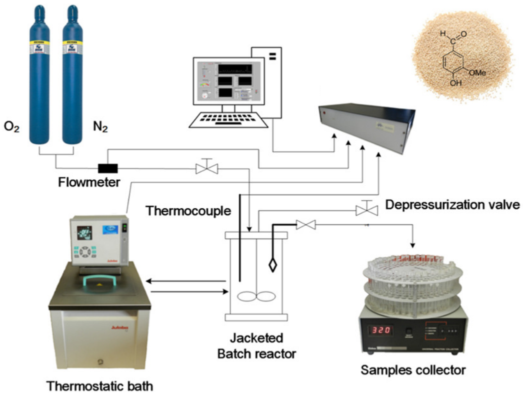
A. Ferreira da Silva[1,2], C. Brazinha[3], L. Costa , N.S. Caetano [1,4]*
[1] LEPABE, Faculty of Engineering, University of Porto, Porto, Portugal; [2]A4F - Algae For Future; [3]LAQV-REQUIMTE, Chemistry Departments, FCT, Universidade Nova de Lisboa, Portugal; [4]School of Engineering (ISEP), Polytechnic of Porto (P.Porto), Porto, Portugal;
** andre.silva@algafuel.pt.*

A Biorefinery is an industrial complex where a single feedstock of biological origin, is transformed into several products in order to obtain the maximum value. Due to the high economic value of certain cellular components, like carotenoids and polyunsaturated fatty acids, microalgae are a very interesting biomass for this application. This project began from the blueprints of two 10 ha large-scale plants, producing two different microalgae strains. For both microalgae strains, different biorefinery scenarios were designed, each one with different sequences of unit operations, equipment and products. With the design stage completed, the economical information from those scenarios will be inserted in GAMS, an optimization program, and used to choose the 3 scenarios with the best economic performance. Afterwards an LCA analysis of the 3 chosen options will be performed in order to assess an optimal and most sustainable biorefinery configuration for both microalgae.

[P-BS17]

Oxidative degradation of vanillin, vanillic acid and acetovanillone

*F. Casimiro**, *C. Costa, A.E. Rodrigues*
Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Department of Chemical Engineering, Faculty of Engineering, University of Porto, Portugal;
** fmacc@fe.up.pt*

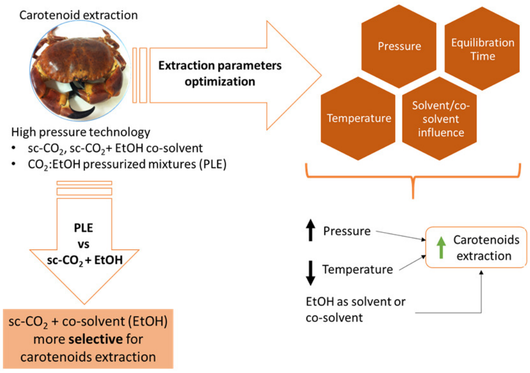


Vanillin (V), vanillic acid (VA) and acetovanillone (VO) are reaction products derived from lignin oxidation. The evaluation of its degradation will enable a better understanding of lignin oxidation reaction, helping to maximize the yields of these target value-added compounds. In this context, the main objective of this work is to study the oxidative degradation of V, VA and VO under the same conditions of lignin oxidation. Oxidation reactions were performed in alkaline medium with oxygen and the effect of temperature (100 - 140 ºC), oxygen partial pressure (2.0 - 5.0 bar) and initial concentration of V, VA and VO (1.25 - 5.0 g/L) was evaluated. The results showed that the different values of initial concentration do not affect V degradation yield; however, the partial pressure of oxygen and the initial temperature increase the degradation of all the phenolic compounds studied.

[P-BS18]

Extraction of carotenoid pigment from brown crab residues using high pressure technology

A. Roda[1] *A. N. Nunes*[1], *A. A. Matias*[1, *]
[1] *iBET, Instituto de Biologia Experimental e Tecnológica, Apartado 12, 2781-901 Oeiras, Portugal*
**amatias@ibet.pt*



The interest in recovering carotenoids from waste products has been growing due to its natural antioxidant and dye properties.

This work focused on the extraction of carotenoids from brown crab residues using high pressure technology.

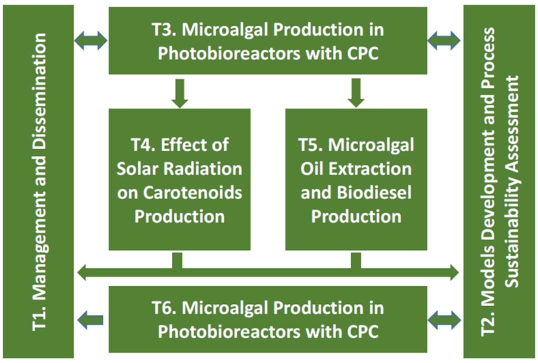
Supercritical CO_2 (sc-CO_2) extractions using 0 to 6% ethanol as co-solvent and pressurized liquid extractions (PLE) with 50-100% EtOH (w/w) were studied to access and optimize the extraction parameters (pressure, temperature, equilibrium time and solvent and co-solvent influence).The process was characterized in terms of total mass yield, carotenoids yield and carotenoids content in the extract.

Within the studied parameters, the carotenoid content increased with pressure and decreased with temperature. Ethanol was found to be crucial for carotenoids extraction, since 100% sc-CO_2 was poorly efficient. Also, sc-CO_2 with co-solvent was more selective for the recovery of carotenoids than the S-L conventional extraction or PLE with EtOH and CO_2.

[P-BS19]

PIV4Algae - Process Intensification for microalgal production and valorisation

J.P. Losa[1], *F.G. Martins*[1], *M.C.M. Alvim-Ferraz*[1], *J.M. Dias*[1], *F.X. Malcata*[1], *R.A.R. Boaventura*[2], *V.J.P. Vilar*[2], *J.C.M. Pires*[1,*]
[1]Laboratory for Process Engineering, Environment, Biotechnology and Energy (LEPABE), Chemical Engineering Department, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465, Porto, Portugal
[2]Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Chemical Engineering Department, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465, Porto, Portugal
** jcpires@fe.up.pt*

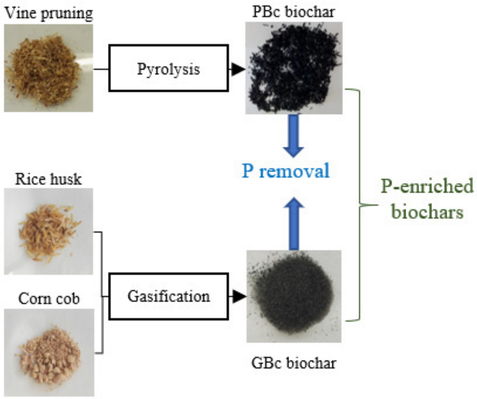


The production and release of N- and P-rich effluents is one of the most serious environmental problems posed by several industries, as this can lead to eutrophication. Tackling this problem, the PIV4Algae project aims at the improvement of a bioremediation strategy using microalgal cultures in which the intensification of biomass production and its valorisation will be under focus.The approach relies on the optimisation of the process parameters for the cultivation of microalgae in existing tubular photobioreactors (PBRs). Modifications of the reactors' hardware are to be tested. After determining the best operating conditions, the biomass will be characterised to assess its potential for oil and carotenoid extraction. The insight provided by these experiments and by CFD (Computational Fluid Dynamics) simulations will allow for the design of an improved PBR system, which will be built at a pilot scale. A techno-economic and sustainability assessment will be performed.

[P-BS20]

Phosphorus adsorption onto biochars from pyrolysis and co-gasification of agricultural biowastes

A. Félix[1], *M. Bernardo*[1], *N. Lapa*[1*], *F. Pinto*[2], *C. Delerue-Matos*[3], *I. Fonseca*[1]
[1]LAQV-REQUIMTE, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal;
[2]Unidade de Bioenergia, Laboratório Nacional de Energia e Geologia, Estrada do Paço do Lumiar 22, Ed. J, 1649-038 Lisboa, Portugal; [3]LAQV-REQUIMTE, Instituto Superior de Engenharia do Porto, Instituto Politécnico do Porto, Rua Dr. António Bernardino de Almeida, 431, Porto, Portugal.
** ncsn@fct.unl.pt*

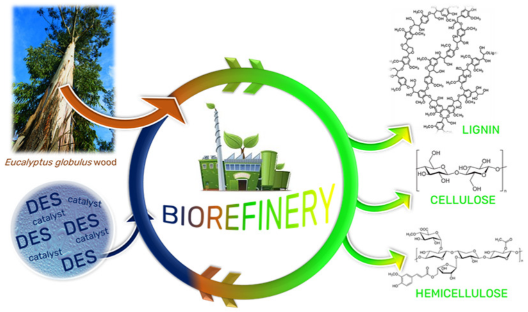


Two different biochars were applied in phosphorus (P) removal from aqueous-phase: one biochar resulting from the pyrolysis of vine prune biowaste (PBc) and another one obtained in the co-gasification of rice husk (RH) with corn cob (CC) (50 % w/w RH + 50 % w/w CC) (GBc). Both biochars were characterized and submitted to P removal assays under different initial pH values (5, 6, 7, 8, 9, 10) to assess the pH influence on chars' P-enrichment. GBc char presented the highest P uptake capacity for all the initial pH values studied, with the best performance of both chars at an initial pH of 9 (uptake efficiency of 25.9 % and uptake capacity of 6.11 mg g^{-1}). PBc also showed its best performance at an initial pH of 9 with a P uptake efficiency of 11.7 % and uptake capacity of 2.62 mg g^{-1}. The higher mineral content of GBc along with its developed porous structure are probably the reasons for the higher P-uptake capacity of this biochar when compared to PBc, for all the initial pH values.

[P-BS21]

Remarkable performance of deep eutectic solvents aqueous solutions on lignin solubilization and wood delignification

B. Soares[1], *A.M. da Costa Lopes*[1], *P.C.R. Pinto*[2], *A.J.D. Silvestre*[1], *C.S.R. Freire*[1], *J.A.P. Coutinho*[1,*]
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal. [2] RAIZ – Forest and Paper Research Institute, Quinta de S. Francisco, 3801-501 Eixo, Portugal;
** jcoutinho@ua.pt*

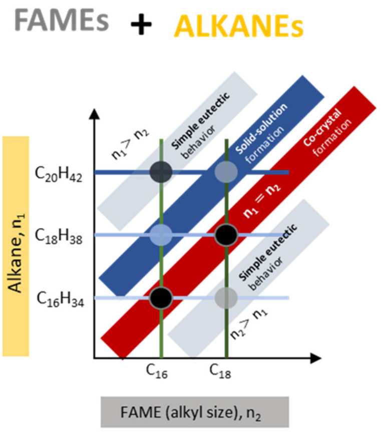


The main goal of this work was to develop Deep Eutectic Solvents (DES) for wood fractionation aiming at their exploitation on pulping processes. To achieve this purpose, fundamental studies were performed to better understand the solubility of lignin model compounds and technical lignins in DES and their aqueous solutions. Particularly, aqueous solutions of propionic acid:urea (PA:U) improved lignin solubility by orders of magnitude in comparison to water and conventional lignin solvents (around 400-fold and 500-fold to kraft lignin and organosolv lignin, respectively). It should be highlighted the fundamental role of water, which mainly governs a hydrotropic effect on lignin solubility in DES aqueous solutions. Finally, the high performance of DES aqueous solutions for wood delignification at mild conditions was also demonstrated. These results are therefore quite promising and might suggest a positive impact on the techno-economic feasibility of the process.

[P-BS22]

Phase behavior of binary mixtures of saturated FAMEs and alkanes

N.F.M. Branco[1,2,3], *J.A.P. Coutinho*[1], *J.C. Ribeiro*[2], *L.M.N.B.F. Santos*[3]
[1]*CICECO, Departamento de Química, Universidade de Aveiro, Aveiro, Portugal;* [2]*GALP, Refinaria de Matosinhos, Porto, Portugal;* [3]*CIQUP, DQB, Faculdade de Ciências da Universidade do Porto, Porto, Portugal*
** nuno.f.m.branco@gmail.com*

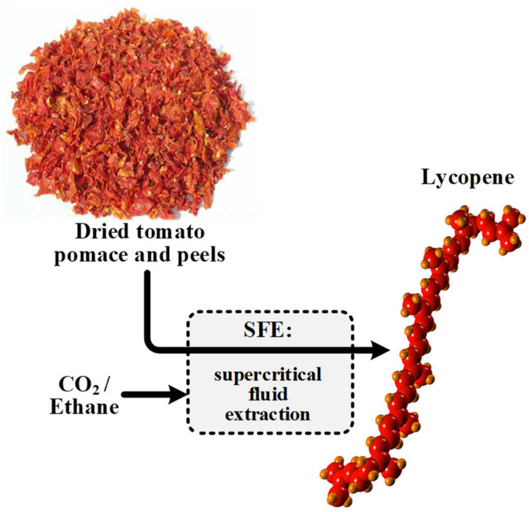


Biodiesel blends with mineral diesel, although improving many characteristics of the fuel and lowering its environmental impact, is detrimental to the low temperature behavior of the diesel. The understanding of the phase behavior of binary mixtures of the main FAMEs present in biodiesel with alkanes in mineral diesel is for great importance to understand, and eventually improve these properties in commercial diesel. This work studied the phase behavior of 6 binary mixtures of a saturated methyl ester with alkanes. These systems show a very complex behavior, with the formation of co-crystals, peritectic reactions, metatectic transitions and the formation of solid solutions. The results here reported show for the first time that in mixtures with equal alkyl chain a co-crystal is formed and the mixtures with an alkane alkyl size two carbon bigger than the FAME lead to the formation of a solid solution increasing the cloud and pour point of the mixture.

[P-BS23]

Life cycle assessment of supercritical fluid extraction of lycopene from tomato residues

M.M. R. de Melo[1,*], *C.M. Silva*[1], *N. Caetano*[2,3], *T. Mata*[2], *A. Martins*[2]
[1]*CICECO, University of Aveiro, 3810-193 Aveiro, Portugal;* [2]*LEPABE, Faculty of Engineering, University of Porto, 4200-465 Porto, Portugal;* [3]*CIETI, School of Engineering (ISEP), Polytechnic Institute of Porto (IPP), 4200-072 Porto, Portugal*
* *marcelo.melo@ua.pt*

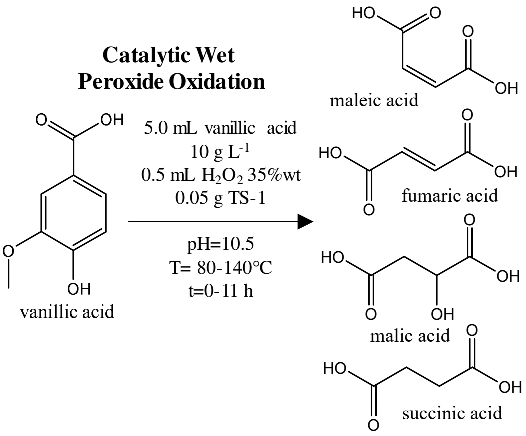


Tomato cultivation and processing is a very relevant agro-industrial activity in a Portuguese context that generates a significant amount of residues, which need to be properly treated and disposed of. One way to valorize the tomato residues is through the extraction of high value compounds, such as lycopene, representing this an extra revenue source. However the selection of the most adequate option should consider their potential environmental impacts. Thus, in this work the supercritical fluid extraction of lycopene from tomato residues is analyzed using a Life Cycle Thinking approach, based on the Life Cycle Assessment (LCA) methodology defined in the ISO 14040. The functional unit is 1 g of lycopene produced from tomato residues. The life cycle stages considered include the transportation and drying of residues, and the lycopene extraction. Inventory data was obtained from process simulations using the AspenTech V7.3 complemented with data from the literature and the Ecoinvent V3.4 LCI database. The results show that the energy consumption, in particular electricity, is the main responsible for the environmental impacts, and the nature of the residue and solvent used have a significant impact on the process environmental performance.

[P-BS24]

Oxidation of vanillic acid for C_4 dicarboxylic acid production in the presence of TS-1 catalyst

C. Vega-Aguilar[1,2], *M.F. Barreiro*[2,3], *A.E. Rodrigues*[1,*]
[1] *LA LSRE-LCM, Department of Chemical Engineering, Faculty of Engineering of University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;* [2] *LA LSRE-LCM, Polytechnic Institute of Bragança, Campus Santa Apolonia Ap 1134, 5301-857 Bragança, Portugal;* [3]*CIMO, Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal.*
* *arodrig@fe.up.pt*



Lignin can be used as a renewable feedstock for the production of C_4 dicarboxylic acids, avoiding the use of petrochemical resources. In this study, vanillic acid, used as a model compound for lignin oxidation, was oxidized using Catalytic Peroxide Wet Oxidation in presence of the TS-1 catalyst, by varying temperature, time and pH. Results showed that vanillic acid was better oxidized under alkaline pH ($pH \geq 9.0$). Moreover, the use of TS-1 catalyst improved the vanillic acid conversion (82-91%), comparatively with the non-catalyzed reaction (16-64%). Also, C_4 acids yield was significantly higher for the catalyzed reaction at $T \leq 120°C$, generating mainly malic, succinic and maleic acids. The reaction was conducted at short times ($t \leq 3.0h$), since longer times promote the acids degradation to lower weight compounds. Vanillic acid behaves similarly to guaiacol oxidation pathway, where maleic acid is the intermediate, being converted to other C_4 acids.

[P-BS25]

Extraction and recovery of phenolic compounds from biomass residues using aqueous solutions of ionic liquids

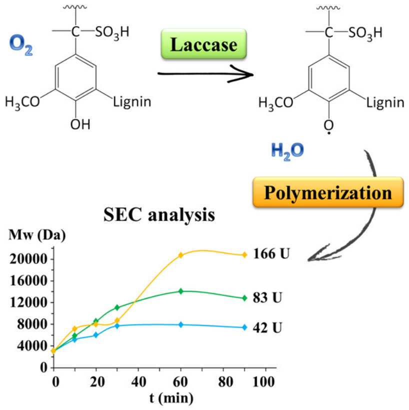
*E.L.P. Faria[1], A.F.M. Cláudio[1], J.A.P. Coutinho, A.J.D. Silvestre[1], M.G. Freire[1]**
[1] CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.
** maragfreire@ua.pt*

Ionic liquids (ILs) have shown to be efficient and alternative solvents to extract a wide variety of compounds from biomass, in which the use of biomass residues plays a pivotal role within a sustainable framework. In this work, we demonstrate the ability of ILs to significantly improve the solubility of syringic acid in water, followed by the use of the most adequate aqueous solutions to extract phenolic compounds from *Rocha* pear peels. An increase in the solubility of syringic acid up to 85-fold was observed in presence of ILs when compared with its solubility in pure water. A response surface methodology was applied to optimize the extraction operating parameters using the best identified ILs, in which extraction yields of syringic acid up to 2.22 wt% were obtained. Finally, it was demonstrated that the target phenolic acid can be recovered from aqueous solutions of ILs by a dilution approach, in which water acts as anti-solvent.

[P-BS26]

Oxidative polymerization of magnesium-based lignosulphonates from acidic *Eucalyptus globulus* sulfite pulping by laccase: preliminary results

S. Magina, A. Barros-Timmons, D.V. Evtuguin*
CICECO – Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal.
** smagina@ua.pt*

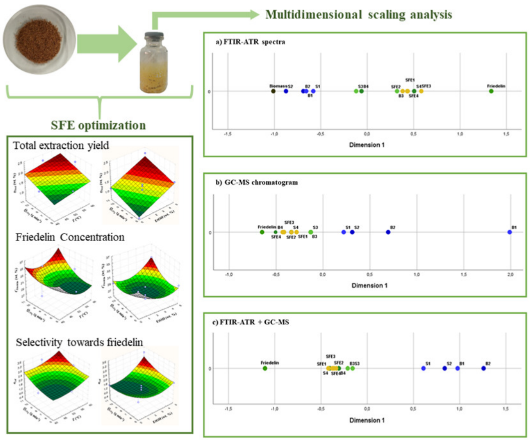


Lignosulphonates (LS) are sulphonated lignin-derived by-products present in sulphite spent liquors (SSL). The valorization of LS represents an important profit for pulp companies and is a challenge towards biorefinery and circular economy concepts. LS are already used in concrete applications as water reducing admixtures. Their plasticizing properties could be enhanced by increasing their molecular weight (Mw) and functionality in order to substitute partially or even completely the superplasticizers from fossil sources. Accordingly, laccase-catalyzed oxidative polymerization of LS from SSL was carried out under pre-selected conditions (temperature, exposure time and enzymatic load) allowing the Mw increase up to 7 folds (from 3240 Da in initial LS to *ca* 21.0 kDa). The modified LS fractions were fairly good soluble in water and contained an increased amount of □-CO groups in conjugated phenolic structures as revealed by the UV-Vis analysis of the modified LS fractions.

[P-BS27]

Valorization of *Quercus cerris* cork by supercritical extraction with modified carbon dioxide as green and efficient solution in relation to the classical extraction with organic solvents

P.G. Vieira[1,*], *M.M.R. de Melo*[1], *A. Şen*[2], *M.M.Q. Simões*[3], *H. Pereira*[2], *I. Portugal*[1], *C.M. Silva*[1]
[1] CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro 3810-193, Portugal; [2] Centro de Estudos Florestais, Instituto Superior de Agronomia, Universidade de Lisboa, Tapada da Ajuda, 1349-017 Lisboa, Portugal; [3] QOPNA, Department of Chemistry, University of Aveiro, Aveiro, Portugal;
** pedro.goncalo@ua.pt*

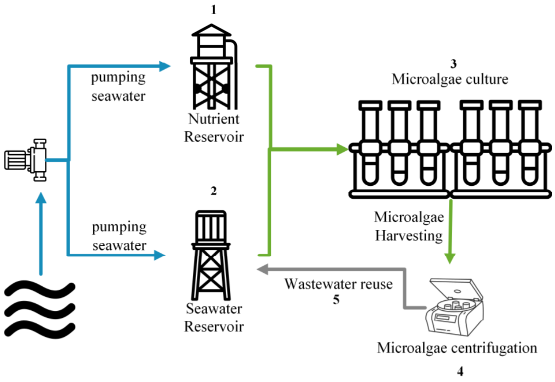


The optimized production and the characterization of extracts from *Quercus cerris* cork using distinct solvents were accomplished in this work. Various extraction methods (batch solid-liquid extraction, Soxhlet extraction, and supercritical fluid extraction (SFE)) and solvents with different polarity (methanol, ethanol, dichloromethane, petroleum ether and modified supercritical carbon dioxide) were compared. The multidimensional scaling (MDS) technique was used to analyze the results, based on GC-MS and FTIR-ATR data. This statistical approach reinforced the proximity between weakly/non-polar extracts and pure friedelin, and between alcoholic extracts and the original biomass. From the SFE optimization, the best conditions that maximize total yield and selectivity towards friedelin were: 60 °C, 5 wt.% EtOH, 11 $\mathrm{g_{CO_2}\,min^{-1}}$. For friedelin concentration in the extracts, the maximum was attained for 40 °C, 0 wt.% EtOH and 5 $\mathrm{g_{CO_2}\,min^{-1}}$. In general, the optimum SFE conditions will always depend on whether an extract enriched in a higher diversity of compounds is preferred, or in a single target molecule like friedelin.

[P-BS28]

Life-cycle inventory analysis of microalgae-based biomass production

M. Branco-Vieira[1,2*], *M. Freitas*[2], *T.M. Mata*[1], *A.A. Martins*[1], *N. Caetano*[1,3]
[1] LEPABE, Faculty of Engineering of University of Porto, 4200-465 Porto, Portugal; [2] Energy Planning Program, Federal University of Rio de Janeiro, 21941-914 Rio de Janeiro, Brazil; [3] CIETI, School of Engineering (ISEP), Polytechnic of Porto (P.Porto), 4200-072 Porto, Portugal;
** monique.branco@fe.up.pt*

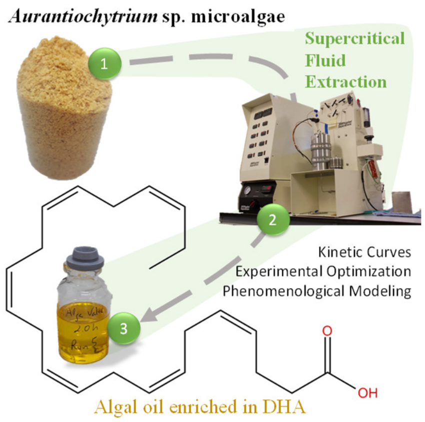


Microalgae have been reported as one of the most promising alternative feedstocks for industrial use. However, the use of microalgae for bioproducts production generates a significant amount of residual biomass, which can be used in integrated biorefineries for the extraction of added-value products. The analysis of the process using the Life-Cycle Assessment (LCA) permits to recognize the best routes and the technological processes with the lowest environmental impact, according to reduction and higher efficiency in feedstock uses. Therefore, in this study it was performed a Life-Cycle Inventory Analysis (LCIA), based on real process data, which was scale-up to a microalgae biomass production industrial plant. Values of energy, nutrients, water and materials consumption were used to create an inventory of inputs and outputs for the biomass production. This approach should support the decision-making, through the identification of critical factors to promote the development of sustainable pilot and large-scale algae-based biorefinery.

[P-BS29]

Valorization of *Aurantiochytrium* sp. microalgae through supercritical fluid extraction: optimization of conditions, measurement and modeling of kinetic curves

M.M.R. de Melo[1,*], *M. Sapatinha*[2], *J. Pinheiro*[3], *M. Lemos*[3], *N.M. Bandarra*[2], *I. Batista*[2], *M.C. Paulo*[4], *J. Coutinho*[4], *J. Saraiva*[5], *C.M. Silva*[1]
[1] CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro 3810-193, Portugal; [2] Division of Aquaculture and Upgrading, Portuguese Institute of the Sea and Atmosphere, Rua Alfredo Magalhães Ramalho, 6, 1495-006 Lisboa; [3] MARE – Marine and Environmental Sciences Centre, School of Tourism and Maritime Technology, Polytechnic Institute of Leiria, 2520-641 Peniche, Portugal; [4] DEPSIEXTRACTA - Tecnologias e Biológicas, Lda, Quinta Taipadas, Canha, Portugal; [5] Department of Chemistry, Research Unit of Química Orgânica, Produtos Naturais e Agroalimentares (QOPNA), University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal.
**marcelo.melo@ua.pt*

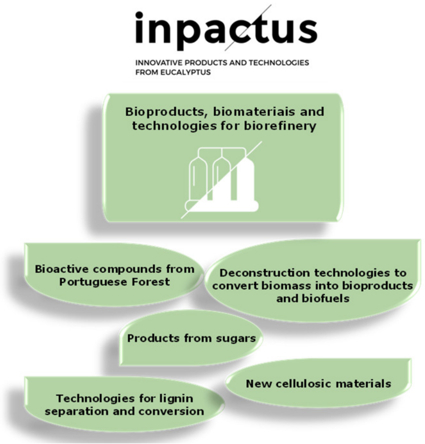


The valorization of *Aurantiochytrium* sp. biomass was accomplished through supercritical fluid extraction (SFE) aiming at the production of algal oil enriched in docosahexaenoic acid (DHA, 22:6 ω3). Pressure, temperature and flow rate conditions were optimized and kinetic curves were measured and modeled. The experimental optimization pointed to 300 bar, 40 ºC, 12 g min^{-1} of CO_2 as the preferable conditions to maximize both η_{total} and x_{DHA}. Under these conditions, $\eta_{\text{total}} = 13.6$ wt.% and $x_{\text{DHA}} = 39.2$ wt.%, with DHA standing as the most abundant individual fatty acid in the extracted oil. The SC-CO_2 modified with 5 wt.% of ethyl acetate is able to boost the extraction rate in the first two hours of extraction, which is confirmed by both the solubility and diffusional parameters fitted using the broken plus intact cells (BIC) model. Overall, the work supports the industrial exploitation of the *Aurantiochytrium* sp. microalgae by SFE for the production of algal oil enriched in DHA.

[P-BS30]

Past and future research programme on biorefinery and bioproducts at the Navigator Company

P.C.R. Pinto[*], *A. Gaspar, R.J. Rodrigues, C.P. Neto*
RAIZ - Forest and Paper Research Institute, Aveiro, Portugal.
** paula.pinto@thenavigatorcompany.com*



The Navigator Company and RAIZ - Forest and Paper Research Institute have been leading research activity in biorefinery, in close collaboration with academic partners and other institutions. Forest biomass, side streams and eucalyptus kraft pulp have been investigated as feedstocks for bioactive extracts, sugars, bio-based chemicals and new materials based on lignin and cellulose. This communication presents the outputs of these projects as the sound basis for the new cycle on R&D in the forthcoming years. The R&D program was recently reinforced by the new collaborative project inpactus - Innovative Products and Technologies from Eucalyptus, involving 14 National and International partners, defining the R&D activities on technologies and processes for the next years. This is an exemplary case of co-promotion R&D project between industry and academia, as a step forward to a green, global, sustainable and competitive bioeconomy in Portugal, based on eucalyptus pulp-and-paper industry.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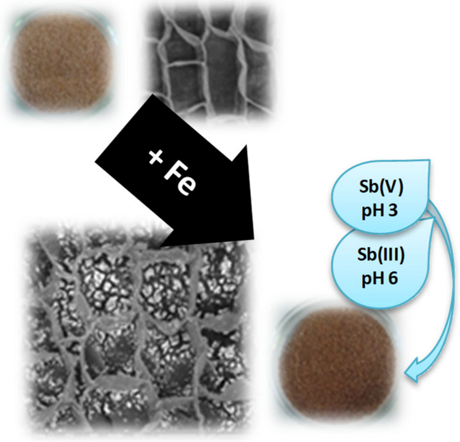
Poster Session

REACTION AND SEPARATION PROCESS

[P-RS01]

Removal of antimony from water by iron-coated cork granulates

A. Pintor, B. Vieira, R. Boaventura, C. Botelho**
Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (LSRE-LCM), Departamento de Engenharia Química, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.
** ampintor@fe.up.pt ; cbotelho@fe.up.pt*

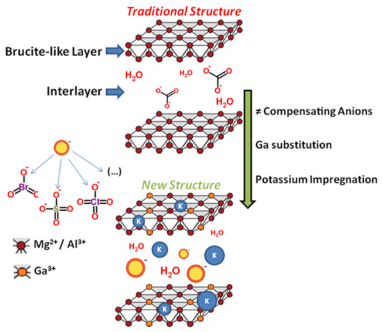


Antimony is a metalloid with similar chemistry to arsenic but whose treatment is not as extensively studied. In this work, removal of antimony in both Sb(III) and Sb(V) oxidation states was performed using iron-coated cork granulates. It was found that Sb(III) adsorption was independent of pH in the range 4-10, while Sb(V) adsorption decreased with pH increase, being optimal at pH 3 when iron leaching was taken into account. Adsorption kinetics were slow for Sb(V) and equilibrium was only approached after 240 h, while for Sb(III) it was reached in about 16 h. The Elovich model fitted well to the experimental data. Both oxidation states followed a Freundlich isotherm for equilibrium data. Affinity was higher for Sb(V) than Sb(III). The Langmuir model allowed the estimation of the maximum adsorption capacities of 5.8 ± 0.5 mg g^{-1} for Sb(III) and 12 ± 2 mg g^{-1} for Sb(V). Iron-coated cork granulates proved to be adequate environmentally friendly adsorbents for Sb removal from water.

[P-RS02]

Study of the effect of the compensating anion on the CO_2 sorption capacity of hydrotalcite-based sorbents

C. Rocha[1], M. Soria[1], L.M. Madeira[1,]*
[1] LEPABE, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, PortugaL.
** mmadeira@fe.up.pt*

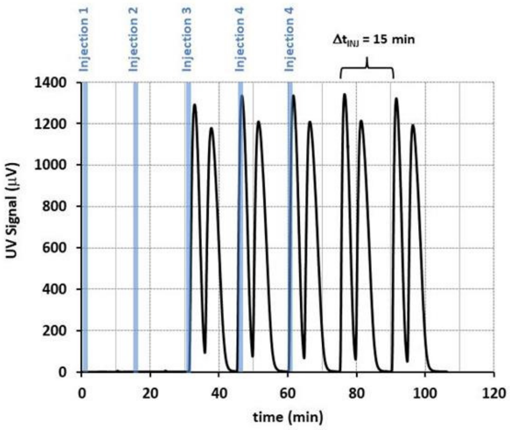


In this work, several hydrotalcites (HTCs) with different compensating anions were prepared to be used as CO2 sorbents. It was found that the type of compensating anion, the partial substitution of Al^{3+} by Ga^{3+} and the impregnation with K_2CO_3 affect the CO_2 sorption capacities of the materials. Besides the physicochemical characterization of the HTCs, the sorption equilibrium isotherms and breakthrough cycles were performed.
It was found that some of the sorbents prepared present very good performance as compared to state-of-art materials, opening the possibility to be subsequently used in a sorption-enhanced reaction process where CO_2 capture improves overall performance.

[P-RS03]

Separation of nadolol racemates by high pH reversed-phase preparative fixed-bed chromatography: Comparison of C18 materials

R. Arafah[1,2], *A. Ribeiro*[1,2], *A. Rodrigues*[2], *L. Pais,*[1,2,*]
[1]*Centro de Investigação de Montanha (CIMO), Polytechnic Institute of Bragança, Campus de Santa Apolónia, Apartado 1134, 5301-857 Bragança, Portugal;* [2]*Laboratory of Separation and Reaction Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal.*
** pais@ipb.pt*

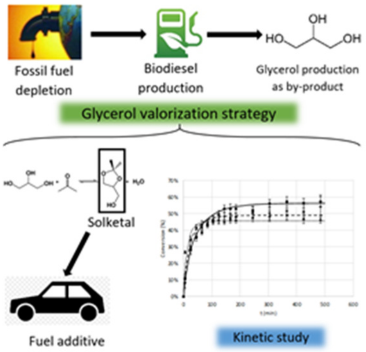


Fixed-Bed technology will be used for the multicomponent preparative separation of a pharmaceutical beta-blocker chiral drug. New strategies using different achiral stationary phases will be presented. Nadolol is a quaternary mixture of equal amounts of four stereoisomers and will be used as case-study. A new methodology for the design, optimization and experimental implementation of the multicomponent separation will be introduced, including the use of three different achiral adsorbents, the screening and choice of the best adsorbent-solvent combination, taking in account the final preparative separation using the fixed-bed technology. Extensive experimental and simulation results will be presented, including solvent screening, measurement of equilibrium adsorption isotherms, breakthrough measurements, and fixed-bed (Azura prep HPLC unit) experimental preparative separation using C18 columns under reversed-phase mode.

[P-RS04]

Solketal production from glycerol ketalization with acetone: Thermodynamic and reaction kinetic study

M.N. Moreira[1], *R.P.V. Faria*[1*], *A.M. Ribeiro*[1], *A.E. Rodrigues*[1]
[1] *Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (LSRE-LCM), Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal.*
**ruifaria@fe.up.pt*

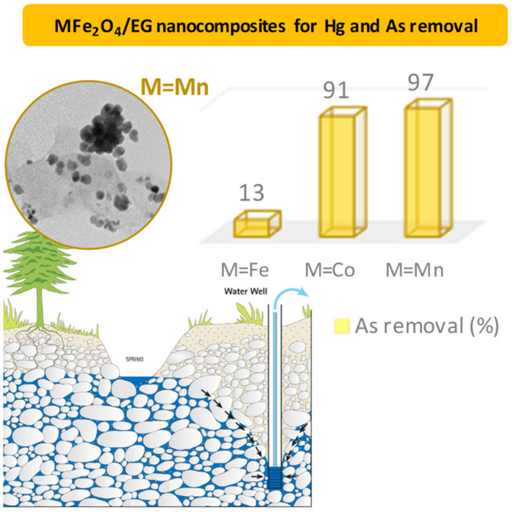


The main results of a thermodynamic and kinetic study of glycerol ketalization to produce solketal in the presence of ethanol, as solvent, are presented in this work, using Amberlyst-35 ion-exchange resin as catalyst for this reaction. Reaction equilibrium and kinetic parameters were determined in a batch reactor, in the absence of external mass transfer limitations. Concerning reaction thermodynamic equilibrium, it was obtained a standard enthalpy of ΔH^0=-13.2± 3.8 kJ mol^{-1}. Eley–Rideal (ER), Langmuir–Hinshelwood–Hougen–Watson (LHHW) and Pseudo-Homogeneous (PH) kinetic models were proposed to fit the obtained experimental data. LHHW reaction rate law could accurately describe the experimental results, considering the presence of internal mass-transfer resistances. The activation energy for the overall reaction was found to be 74.7 ± 17.0 kJ mol^{-1}.

[P-RS05]

Spinel type – carbon based nanocomposites for the magnetically assisted removal of Hg and As species from different aqueous matrices

R. de Groot [1], D. Tavares[2], E. Pereira[2], T. Trindade[3], N. Hartog[1]. C.B. Lopes[3,4,]*
[1] University of Utrech, Netherland; [2] CESAM, University of Aveiro, 3810-193 Aveiro, Portugal, Portugal; [3]CICECO, University of Aveiro, 3810-193 Aveiro, Portugal, [4] CIIMAR, 4450-208 Matosinhos, Portugal.
** claudia.b.lopes@ua.pt*

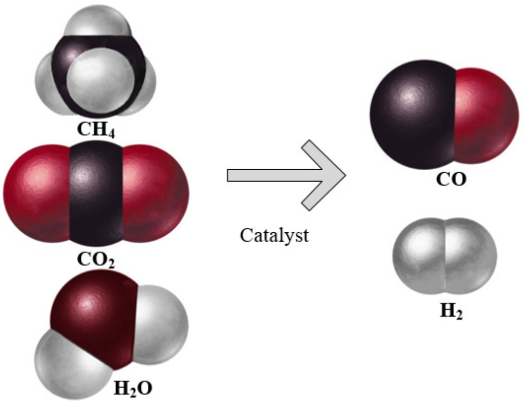


Six magnetic composites were synthesized by two methods, using 3 types of spinel ferrites (SF: MFe_2O_4 M=Fe, Co or Mn) and exfoliated graphite(EG). In the first method(EG1), the SFs were synthesized prior to addition to EG and the composites were prepared by electrostatic assembly, while in the second one (EG2), the SFs were synthesized in the presence of EG by in situ oxidative hydrolysis process. The composites were studied as sorbents for the removal of two toxic elements (As and Hg), from different aqueous matrices. The removal efficiency of all composites was evaluated in batch conditions, at Hg and As wastewater guideline concentration, at pH 6. In general, most Hg removal was seen for the SF@EG1 composites, while most As removal was seen for the SF@EG2 composites. The lowest Hg and As removal was seen for all the Fe_3O_4 materials. As a proof of concept, composites were applied in As contaminated groundwater, and >90% removal was seen for both $CoFe_2O_4$@EG2 and $MnFe_2O_4$@EG2.

[P-RS06]

Carbon dioxide ennoblement via catalytic bi-reforming of methane

A.F. Cunha [1,], T.M. Mata[2], N.S. Caetano[2,3], A.A. Martins [2], J.M. Loureiro[1]*
[1] LSRE/LCM, FEUP, R. Dr. Roberto Frias S/N, 4200-465 Porto, Portugal; [2] LEPABE/FEUP, R. Dr. Roberto Frias S/N, 4200-465 Porto, Portugal; [3] ISEP R. Dr. António Bernardino de Almeida 431, 4249-015 Porto, Portugal.
** afcunha@fe.up.pt*

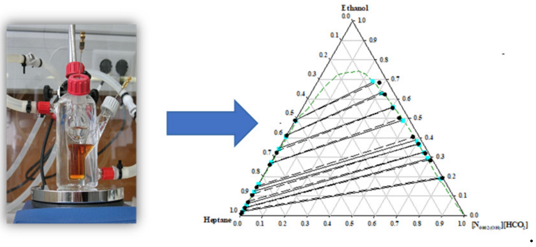


To minimize the impacts resulting from increasing emissions of greenhouse gases, in particular carbon dioxide and methane, there is a need to develop new processes that may reduce net carbon emissions and contribute to a more circular economy. Bi-reforming of methane (BRM) is a promising method for syngas production, with a hydrogen-to-carbon monoxide ratio of two, relevant for example, when the purpose is methanol synthesis. In this work, reaction studies were carried out over a nickel-based catalyst varying the temperature (798-1123 K). Results show that synthesis gas can be successfully produced using this process. For the range of operating conditions studied, the carbon dioxide and methane conversions increase with temperature, reaching 100 % and 40 %, respectively. Future work will analyze the influence of other factors, in particular using higher amounts of catalyst or different feed mixtures, with the goal of approximating the hydrogen-to-carbon monoxide ratio to levels more suited for methanol production.

[P-RS07]

Separation of azeotropic mixtures with aprotic solvents

*J.E. Sosa[1], J.M.M. Araújo[1], E. Amado-González[2], A.B. Pereiro[1,]**
[1]LAQV, REQUIMTE, Department of Chemistry, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal; [2]Faculty of Chemistry, University of Pamplona, Pamplona, Colombia
**anab@fct.unl.pt*



One of the most problems in the industrial processes is the presence of azeotropic or close-boiling mixtures because their separation is impossible by distillation. In this work, aprotic ionic liquids (2-hydroxyethylammonium formate, [$N_{0002(OH)}$][HCO_2], 2-hydroxyethylammonium propanoate, [$N_{0002(OH)}$][$C_2H_5CO_2$], and 2-hydroxyethylammonium butyrate, [$N_{0002(OH)}$][$C_3H_7CO_2$]) are proposed to be used as extraction solvents in liquid-liquid extraction processes. The separation of n-hexane and n-heptane from azeotropic mixtures with ethanol was analysed using the liquid + liquid equilibrium for different ternary systems at 298.15 K and atmospheric pressure. NRTL model was used to correlate the experimental data with Aspen Plus V.9. The results suggest that the extraction of ethanol from the azeotropic mixtures is possible in both systems. The ionic liquid that showed the best results was [$N_{0002(OH)}$][HCO_2]. This ionic liquid can separate these azeotropic mixtures, showing a great potential to replace the organic solvents in

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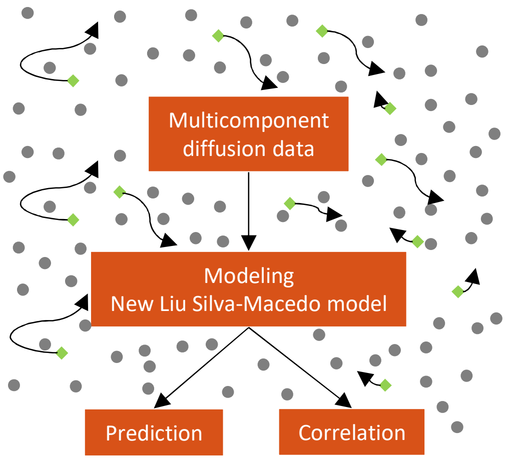
[P-RS08]

New extension of the Liu-Silva-Macedo model to multicomponent Lennard-Jones intradiffusivities

*B. Zêzere[1], I. Portugal[1], C. M. Silva[1,]**
[1] CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro 3810-193, Portugal
**carlos.manuel@ua.pt*



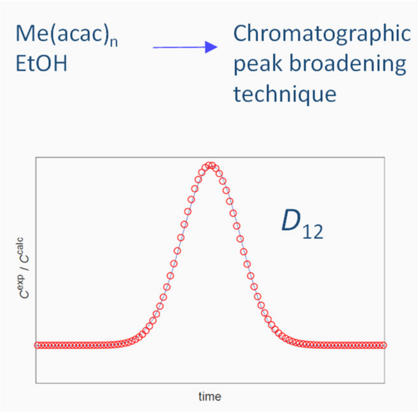
Transport properties such as molecular diffusion coefficients (D_{12}) are very important for the accurate design and optimization of industrial processes involving mass transfer. However, there is a lack of experimental diffusion coefficients, especially for multicomponent systems, and accurate models for D_{12} estimation.

In this work, a new extension of the Liu-Silva-Macedo model to multicomponent Lennard-Jones intradiffusivities (New-LSM) is presented. The model was devised and the embodied parameters optimized using a database containing 1457 experimental points spanned across 131 ternary systems. Two model variants were developed, one for prediction and another for correlation. The New-LSM predictive model achieved an average relative deviation of 7.93 % that range from 0.73 to 41.34 %, while the New-LSM 1-parameter correlation attained an average deviation of 4.15 % ranging from 0.23 to 15.75 %.

[P-RS09]

Experimental and modeled diffusivities of metal acetylacetonates in liquid ethanol, and comparative insights with their diffusivity in supercritical CO_2

B. Zêzere[1], I. Portugal[1], C.M. Silva[1,]*
[1]CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro 3810-193,Portugal
**carlos.manuel@ua.pt*

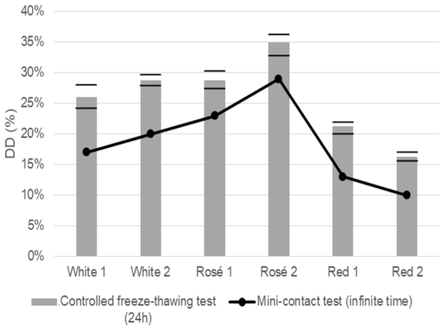


Diffusion coefficients (D_{12}) are important for the modeling, design and optimization of rate-controlled processes. In this essay, the D_{12} of five metal acetylacetonates ($\mathrm{Me(acac)}_n$), namely palladium(II) acetylacetonate, chromium(III) acetylacetonate, vanadyl(II) acetylacetonate, nickel(II) acetylacetonate and titanium(IV) oxyacetylacetonate, were measured in liquid ethanol using the chromatographic peak broadening technique. The measurements were performed at atmospheric pressure at temperatures between 303.15 and 333.15 K. The obtained D_{12} values ranged from 0.789×10^{-5} to 2.00×10^{-5} $\mathrm{cm^2\ s^{-1}}$. Furthermore, our D_{12} values in ethanol were compared with the corresponding $\mathrm{Me(acac)}_n$ in supercritical CO_2 (SC-CO_2) compiled from the literature. Both SC-CO_2 and ethanol data were modeled with well-known literature equations, having achieved relative deviations from 0.32 to 34.71 %.

[P-RS10]

A new test to measure the degree of deionization required for tartaric stabilization of wines by electrodialysis

P. Henriques[1,], V. Geraldes[1], A. M. Brites Alves[1]*
[1] Instituto Superior Técnico, Chemical Engineering Department, Center of Physics and Engineering of Advanced Materials, Avenida Rovisco Pais, 1, 1049-001 Lisbon, Portugal.
** patricia.henriques@tecnico.ulisboa.pt*

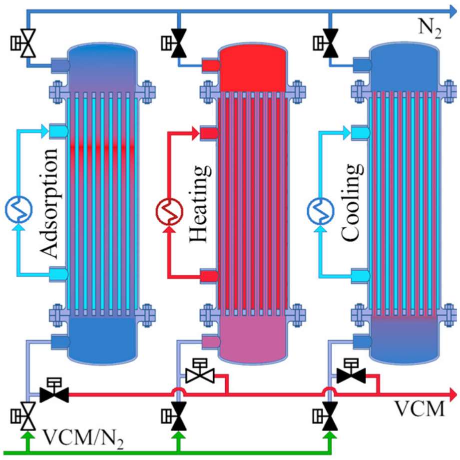


In this work, a controlled freeze-thawing test for the evaluation of the deionization degree (DD), which is associated to wine tartaric stabilization by electrodialysis, is proposed. Wine samples are frozen at -20ºC in a single direction, from bottom to top, thereby ensuring their controlled nucleation, maintained frozen for 24 hours and finally thawed at 0ºC. Results of this test were compared with those obtained from the well-known mini-contact test. The deionization degrees obtained with the mini-contact test show an under-prediction between 5 and 9% when compared to the new test. Based on these results this new method proved to be more reliable and reproducible than the mini contact test, giving more precise DD values to be used as a set-point in the tartaric stabilization of wines by electrodialysis.

[P-RS11]

Packed shell and tube heat exchanger for the separation and recovery of unreacted monomer in polyvinyl chloride plants

P.M. Carmo[1,*], *A.M. Ribeiro*[1], *A.E. Rodrigues*[1], *A.F.P. Ferreira*[1]
[1] *Laboratory of Separation and Reaction Engineering Associated Laboratory, LA/LSRE-LCM, Faculdade de Engenharia Universidade do Porto, Rua Dr. Roberto Frias 4200-465, Porto, Portugal;*
**paulo.carmo@fe.up.pt*

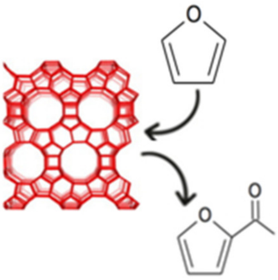


Most of the produced vinyl chloride (VCM) is used in the polymerization towards polyvinyl chloride (PVC). As this reaction does not have a total conversion, the unreacted monomer must be purged from the reaction slurry, purified, and recycled back to the polymerization reactor. This monomer recovery gives answer to both economical, and health and safety requirements. In this work, a 2-dimensional (2D) mathematical model of a Temperature Pressure Swing Adsorption (TPSA) was developed for the equilibrium adsorption separation of VCM and nitrogen (N_2), on activated carbon. In order to increase the process heat transfer rate, a shell and tube geometry was studied and implemented into the TPSA model. Using this geometry, a 5-step system of 3 adsorbent packed shell and tube heat exchangers was designed to separate and purify a 40:60 % (v/v) VCM/N_2 gas mixture. This system was designed to produce a 95 % (v/v) VCM rich stream and a N_2 stream with a VCM limit concentration of 8 ppm (w/w).

[P-RS12]

Catalytic performance of rare-earth doped HBEA zeolites over Friedel-Craft acylation reactions

L. Borbinha[1], *N. Nunes*[1,2*], *A. Martins*[1,2], *F. Martins*[1]
[1] *Centro de Química e Bioquímica, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade de Lisboa, Ed. C8, Campo Grande 1749-016 Lisboa, Portugal;* [2] *Área Departamental de Engenharia Química, Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, R. Conselheiro Emídio Navarro, 1, 1959-007 Lisboa, Portugal*
**nnunes@deq.isel.ipl.pt.*

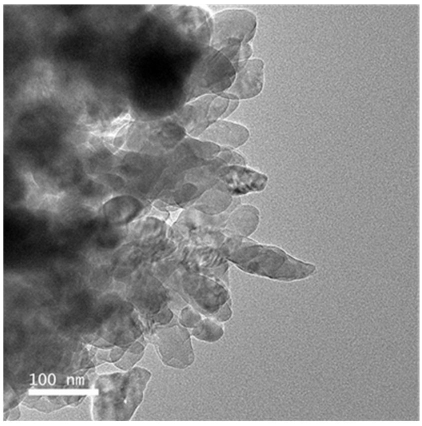


In this work a comparison of the catalytic performance of HBEA zeolite, doped with different percentages of rare-earth cations, in the Friedel-Crafts acylation of furan with acetic anhydride is performed. Kinetic /equilibrium constants were obtained from the mathematical treatment of experimental results with a previously proposed simplified version of the Langmuir-Hinshelwood model. Kinetic constants were also correlated with earlier characterization data of these zeolites namely with Brönsted acidity, quantified by pyridine adsorption followed by FTIR, and catalytic acidity estimated by the model catalytic cracking of *n*-heptane.

[P-RS13]

Effect of dispersant on the stabilization of calcium carbonate nanoparticles

C.F. Almeida[1], Y.A. Manrique[1], J.C.B. Lopes[1,*], M.M. Dias[1]
[1] Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (LSRE-LCM), Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal,
*lopes@fe.up.pt

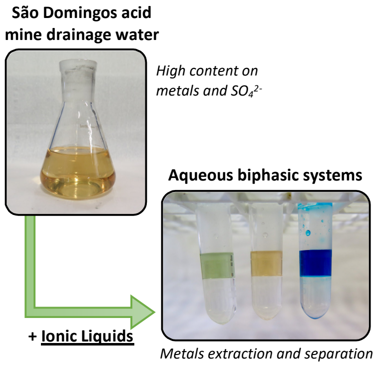


In this work, the effects of the temperature and of different dispersants on the stability over time of a suspension of calcium carbonate nanoparticles were studied. A full recrystallization was obtained, for both analysed temperatures (7 and 20 °C), at the end of one week when the nanoparticles were in a suspension of distilled water. The use of dispersants improved the stability of the suspension. For the case where a sodium citrate solution was used a clear improvement on the particles' stability was observed: at 7 °C, recrystallization of the particles was practically non-existent after 3 weeks; however, a total recrystallization occurred by week 16. A twice more concentrated solution of sodium citrate, at 7 ºC, prevented recrystallization for a minimum of 16 weeks. For a storage solution of sodium oleate, stability was achieved for, at least, 16 weeks. Furthermore, it was seen that lower temperatures had a retarding effect on the recrystallization of the particles.

[P-RS14]

Extraction and recovery of valuable metals from São Domingos acid mine drainage water

H. Passos[1,*], B. Cruz[1], N. Schaeffer[1], C. Patinha[2], E.F. da Silva[2], J.A.P. Coutinho[1]
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Portugal; [2] GeoBioTec, Geoscience Department, University of Aveiro, Portugal.
* hpassos@ua.pt

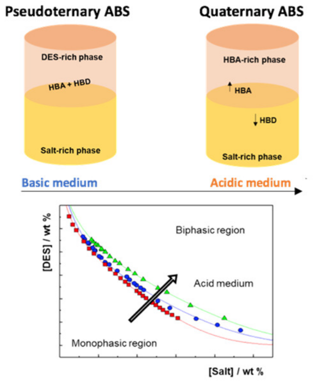


In line with the principles of a circular economy, the development of processes that allows not only the environment detoxification but also the recycling of wastes streams for the recovery of valuable metals is of high relevance. In this work, ionic-liquid-based aqueous biphasic systems (IL-based ABS) were used as a more benign alternative to conventional liquid-liquid extraction processes in metals recovery from acid mine drainage water from São Domingos mine, Portugal. ABS composed of different ILs and Na_2SO_4 were evaluated for metals extraction in both metal standard aqueous solutions and real mine water samples. It was observed that ILs anion presents an important role in metals extraction. Furthermore, it was demonstrated the potential use of conventional salts as additives in IL-based ABS, allowing the increase of the extraction efficiency and selectivity.

[P-RS15]

Deep-eutectic-solvents-based aqueous biphasic systems: The pH effect

F.O. Farias[1], *<u>H. Passos</u>*[2,*], *J.A.P. Coutinho*[2], *M.R. Mafra*[1]
[1] *Department of Chemical Engineering, Federal University of Paraná (UFPR), Polytechnic Center, 81531-990, Curitiba-PR, Brazil.*; [2] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Portugal.*
* *hpassos@ua.pt*

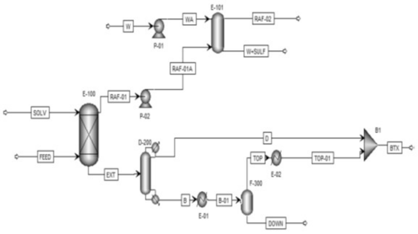


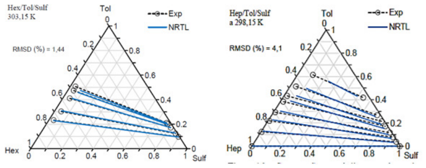
Deep eutectic solvents (DES) are an emerging type of green solvents that have been applied as phase forming components of aqueous biphasic systems (ABS). Here the pH influence on the phase equilibrium and DES' components stoichiometry on the phases of ABS composed of DES (formed by tetrabutylammonium chloride and ethanol or *n*-propanol, at different molar ratio) and potassium citrate/citrate buffer was evaluated at 298 K and pH 9, 7 and 5. In addition the partition coefficients of gallic acid, caffeine and L-tryptophan were also determined, allowing to infer on potential application of these systems. The results suggest that the change on the pH results in the chemical speciation of the potassium citrate salt, and consequently its ability to form an ABS is affected, allowing to control the stoichiometric partition of DES' components and tuning the biomolecules partition behavior.

[P-RS16]

Computational simulation of the aromatic extraction process: Evaluation of thermodynamics and sulfolan selectivity

<u>I.R.S. Araujo</u>[1*], *C.P.G. Lira*[2], *A.E.X. Stragevitch*[3]
[1,2,3] *Laboratory of fuels- Federal University of Pernambuco, Recife, Brazil.*
[*] *italo-araujo@outlook.com*



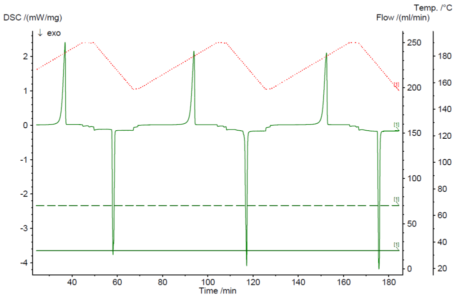


In the aromatic extraction operation, a combination of operations is required to obtain products with a high degree of purity. Aromatic hydrocarbons are obtained from the cut range of naphtha. In general, the target of the extraction is called BTX's (Benzene, Toluene and Xylene) and one of the solvents most used in the process is sulfolane. A unit of aromatic extraction was simulated based on the parameters reported in the literature, using as solvent the sulfolane in the ratio of 1.6 (Solvent/Feed). The conceptual design was carried out with the simplification of the feed with the objective of thermodynamic evaluations and solvent efficiency. The creation of a database with parameters of binary interaction was carried out to characterize the best model to be used in the simulation, excelling NRTL model. A stream of aromatics was obtained in 97% purity. The selectivity of the solvents was evaluated in relation to the solutes of interest, revealing the high potential of the solvent.

[P-RS17]

Studies on the solubility of syringic, vanillic and veratric acids in water and organic solvents

S.M. Vilas-Boas[*], *R.S. Alves, S.P. Pinho, O. Ferreira*
Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal; Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Polytechnic Institute of Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal.

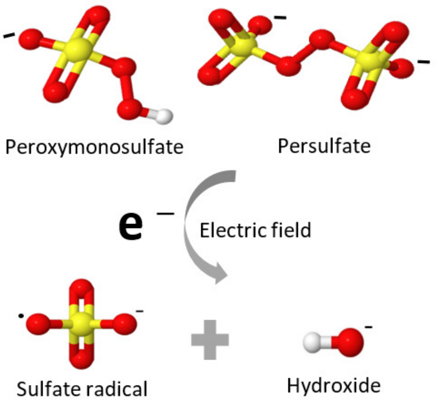


Phenolic acids are a chemical family of significance in the health and food industries, among others. Despite its importance for the design of separation processes, solubility data of phenolic acids are seldom available in literature. In this context the solubility of syringic, vanillic and veratric acids was measured in water and eight organic solvents (methanol, ethanol, 1-propanol, isopropanol, ethyl acetate, acetonitrile, 2-butanone and dimethylformamide) at 298.15 K and 313.15 K using the isothermal analytical shake-flask method. Calorimetric studies were also carried out by differential scanning calorimetry (DSC) to determine the melting properties of the phenolic acids. Finally, the semi-predictive Non-Random Two-Liquid Segment Activity Coefficient (NRTL-SAC) model [1], combined with the reference solvent approach (RSA) [2], was applied to correlate and predict the solid-liquid equilibria. The average relative deviations were 30% for the correlation and 44% for the predictions.

[P-RS19]

Activation of persulfate and peroxymonosulfate by heterogeneous catalysis for the degradation of organic pollutants

M. Arellano[*], *M. A. Sanromán, M. Pazos*
Department of Chemical Engineering, University of Vigo, Isaac Newton Building, Campus As Lagoas-Marcosende, 36310 Vigo, Spain.
** marellano@uvigo.es*

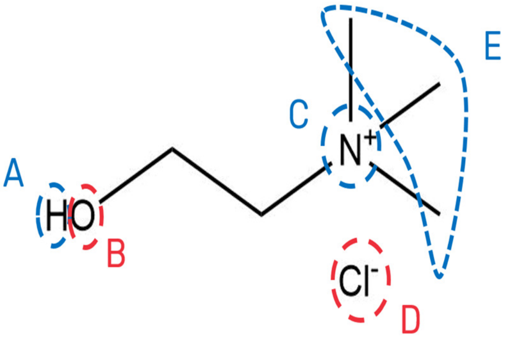


The activation of persulfate and peroxymonosulfate to generate sulfate radicals and degrade organic pollutants was evaluated. The selected pollutants were a dye, Lissamine Green B, and an ionic liquid, 1-butyl-1-methylpyrrolidinium chloride. The key parameters were optimized and both homogeneous and heterogeneous catalysis were assessed, getting better results with the second mode. For the persulfate activation, iron adsorbed in amberlite was used as catalyst. Different concentrations of iron were tested, achieving the best results with 5 g of catalyst (93% of dye removal). For the peroxymonosulfate activation, a system combining iron and electric field was evaluated. The concentration and source of iron (pyrite, goethite and magnetite), the oxidant dosage and the current applied were studied. A TOC decay of 80% was obtained with the activation of peroxymonosulfate (10 mM) with pyrite (1 mM of iron) at 150 mA within 300 min. Moreover, the reusability of both catalysts was demonstrated.

[P-RS21]

Development of a molecular model for [Ch]Cl aiming at the thermodynamic modelling of deep eutectic solvents

E.A. Crespo[*1], *L.P. Silva*[1], *P.J. Carvalho*[1], *L.F. Vega*[2], *F. Llovell*[3], *J.A. P. Coutinho*[1]
[1] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 – Aveiro, Portugal;* [2] *Gas Research Center and Chemical Engineering Department, Khalifa University of Science and Technology (KUST) – The Petroleum Institute, P.O. Box 2533, Abu Dhabi, United Arab Emirates.* [3] *Department of Chemical Engineering and Materials Science, IQS School of Engineering, Universitat Ramon Llull, 08017, Barcelona, Spain;*
** eacrespo@ua.pt*

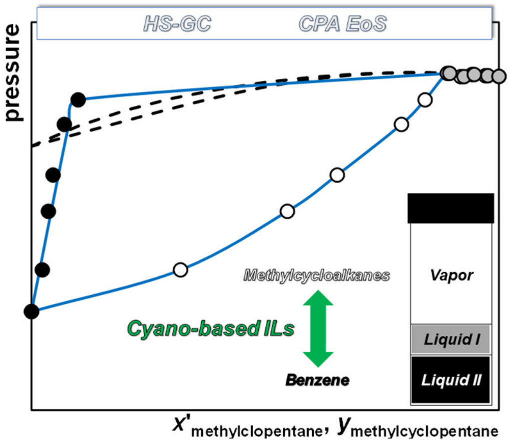


The glut of literature on DESs applications has not been followed by a similar efforted aimed at understanding their nature. This lack of information has been hindering the development of accurate thermodynamic models for DESs which are required for the accurate simulation and design of any industrial process. Molecular based equations of state (EoSs) due to their capability to explicitly account for hydrogen-bonding, have been proposed to model DESs but their application to high-temperature melting salts like those used to form DESs is a non-trivial task. Therefore, in this work, a new coarse-grained model for [Ch]Cl is proposed within the framework of soft-SAFT EoS overcoming the existent limitations. The new model was shown to be able to successfully describe thermophysical properties and phase equilibria of different [Ch]Cl-based DESs without hassle.

[P-RS22]

Methylcycloalkane/benzene separations by extractive distillation with ionic liquids

P. Navarro[1,2*], *M. Ayuso*[3], *A.M. Palma*[1], *M. Larriba*[3], *N. Delgado-Mellado*[3], *J. García*[3], *F. Rodríguez*[3], *J.A.P. Coutinho*[1], *P.J. Carvalho*[1]
[1] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;*
[2]*Departament of Chemical Engineering, Autónoma University of Madrid, c\Francisco Tomás y Valiente 7. 28049 Madrid, Spain;*
[3]*Departament of Chemical Engineering and Materials, Complutense University of Madrid, Avda. Complutense s/n, 28040 Madrid, Spain*
** pntejedor@ua.pt.*

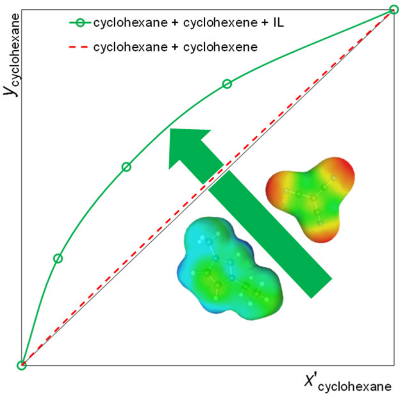


Ionic liquids (ILs) are potential neoteric solvents to design new advanced separation processes. Among several separation cases studied so far, the good performance of ILs regarding the dearomatization of liquid fuels has received especially attention. However, liquid-liquid extraction alone seems not to be enough to fulfill current aromatic commercial standards, i.e. extreme aliphatic and aromatic purities. Extractive distillation with ILs stands as a new process configuration to overcome these limitations by enhancing the aliphatic/aromatic relative volatilities. In this work, a complete experimental and modelling study is presented to further explore extractive distillation with ILs for methylcycloalkane/benzene challenging separations.

[P-RS23]

Cyclohexane/cyclohexene separation by extractive distillation with cyano-based ionic liquids

P. Navarro[1,2,*], *A. Ovejero*[3], *N. Delgado-Mellado*[3], *A.M. Palma*[1], *M. Ayuso*[3], *M. Larriba*[3], *J. García*[3], *F. Rodríguez*[3],
J.A.P. Coutinho[1] *P.J. Carvalho*[1]
[1] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;*
[2]*Departament of Chemical Engineering, Autónoma University of Madrid, c\Francisco Tomás y Valiente 7. 28049 Madrid, Spain;*
[3]*Departament of Chemical Engineering and Materials, Complutense University of Madrid, Avda. Complutense s/n, 28040 Madrid, Spain.*
**pntejedor@ua.pt.*

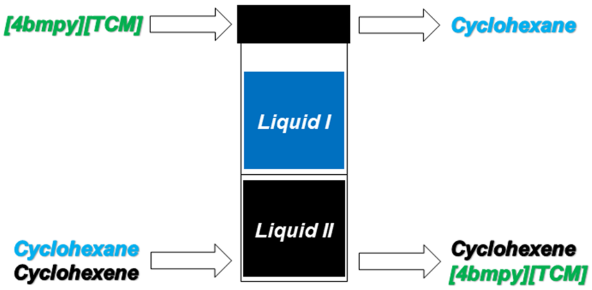


Among other relevant separations for the petrochemical industry, cyclohexane/cyclohexene separation is one of the most costly. Several efforts are destined to enhance separation techniques. In this context, ionic liquids (ILs) are being proposed as interesting solvents due to their special features, i.e. non-volatile character and suitable extractive and physical properties. However, current liquid-liquid extraction technologies based on ILs are not able to reach a feasible technology due to the low cyclohexane/cyclohexene selectivity and cyclohexene distribution ratios. In this context, extractive distillation with ILs stands as an enhancer technology to improve the separation standards and reduce the solvent demand. Among other cyano-based ILs tested in this work, 1-ethyl-3-methylimidazolium tricyanomethanide ($[C_2C_1im][TCM]$) has been revealed as the most promising mass agent.

[P-RS24]

Separation of cyclohexene from cyclohexane by liquid-liquid extraction with ionic liquids

M. Ayuso[1], *N. Delgado-Mellado*[1], *A. Ovejero-Pérez*[1], *P. Navarro*[2,3], *M. Larriba*[1], *J. García*[1,*], *F. Rodríguez*[1],
[1] *Departament of Chemical Engineering and Materials, Complutense University of Madrid, Avda. Complutense s/n, 28040 Madrid, Spain;* [2] *Departament of Chemical Engineering, Autónoma University of Madrid, c\Francisco Tomás y Valiente 7. 28049 Madrid, Spain;* [3] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.*
** jgarcia@ucm.es*

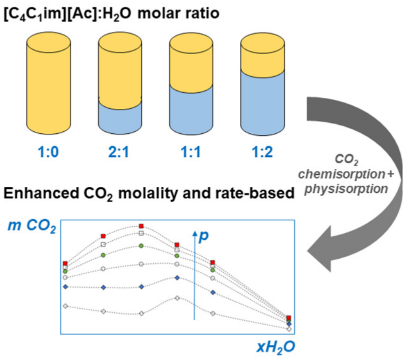


Finding an energy-efficient process for the separation of olefins from paraffins is one of the major challenges in the petrochemical industry. Currently, extractive distillation is the most used technology due to the close boiling points of these compounds; however, this process has several drawbacks and large energetic consumption. Liquid-liquid extraction with ionic liquids (ILs) can overcome these limitations due to the mild operating conditions of this technology and the unique properties of ILs. Five promising ILs have been tested here in the cyclohexane/cyclohexene separation by liquid-liquid extraction. The liquid-liquid equilibria (LLE) for the ternary mixtures {cyclohexane + cyclohexene + IL} were determined at optimized temperatures and atmospheric pressure, regressing the data to Non-Random Two Liquids (NRTL) model.

[P-RS25]

Impact of water on the CO_2 solubility in $[C_4C_1im][Ac]$

P. Navarro[1,2], *<u>P.J. Carvalho</u>*[1,*], *J.A.P. Coutinho*[1]
[1] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal*
[2] *Departament of Chemical Engineering, Autónoma University of Madrid, c\Francisco Tomás y Valiente 7. 28049 Madrid, Spain*
**quijorge@ua.pt.*

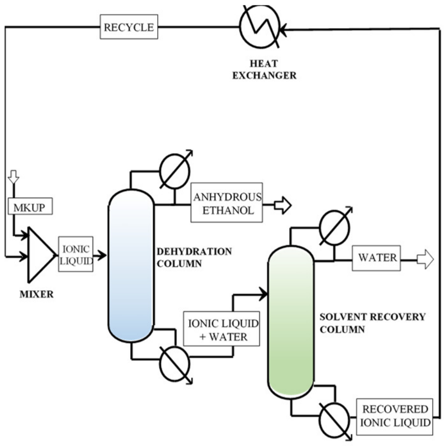


It is widely accepted that the presence of water, even at very low concentrations, have a negative impact on the carbon dioxide solubility in ionic liquids (ILs) but, few studies have focused on evaluating water real impact on the sorption capability over the entire concentration range. Here, the water impact on the CO_2 solubilities in the promising 1-butyl-3-methylimidazolium acetate ($[C_4C_1im][Ac]$) IL was evaluated for $[C_4C_1im][Ac]:H_2O$ molar ratios of 5:1, 2:1, 1:1, and 1:2, for temperatures ranging from (293 to 363) K and pressures up to 70 MPa. Water is shown to improve the IL capability to solubilize CO_2, with equimolar molar ratios leading to enhanced solubilities for pressures up to 5 MPa, whereas $[C_4C_1im][Ac]:H_2O$ molar ratios of 5:1 and 2:1 present higher CO_2 solubility at higher pressures.

[P-RS26]

Simulation and optimization of the ethanol dehydration process by extractive distillation using imidazolium-based ionic liquids as solvents

<u>C. J. Cavalcanti</u>[1*], L. Stragevitch[1], F.R. Carvalho[1], M.F. Pimentel[1]
[1]*Federal University of Pernambuco, Department of Chemical Engineering, Recife-PE, Brazil*
<u>*claudia.jessicacavalcanti@ufpe.br</u>

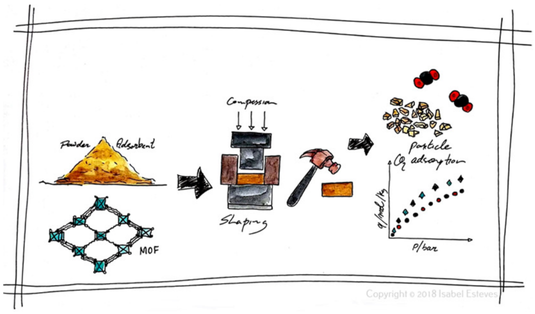


Ionic liquids (ILs) represent a new class of solvents as promising surrogates to conventional organic solvents (volatile and toxic) as well as alternatives to reduce environmental pollution. One use of ILs of great importance to industry is in breaking azeotropes, as in the separation of ethanol/water mixtures. In this work, the extractive distillation process to produce dehydrated ethanol was evaluated for three imidazolium-based ILs as solvents, namely [Emim][Cl], [Bmim][Cl] and [Hmim][Cl]. The Aspen Plus® software was used to simulate the process and multivariate statistical techniques were employed to optimize the separation. The multivariate statistical techniques were effective in the optimization of the process as operational conditions could be determined to minimize the energetic consumption while holding ethanol purity according to specification (greater than 99.3%).

[P-RS27]

Binderless shaped metal-organic framework particles

R.P.P.L. Ribeiro[1,*], *C.L. Antunes*[1], *A.U. Garate*[1], *A.F. Portela*[1], *M.G. Plaza*[2], *J.P.B. Mota*[1], *I.A.A.C. Esteves*[1,*]
[1] *LAQV-REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal;* [2] *Instituto Nacional del Carbón, INCAR-CSIC, C/Francisco Pintado Fe 26, 33011 Oviedo , Spain;*
** rpp.ribeiro@fct.unl.pt ; iaesteves@fct.unl.pt*



Metal-organic framework (MOF) particles were shaped by binderless mechanical compression of commercial ZIF-8 and MIL-53(Al) powders. Two compression pressures were employed — 62 MPa and 125 MPa. The impact in the mechanical, structural, and textural characteristics of the MOFs was evaluated, as well as the influence in carbon dioxide (CO_2) adsorption capacity at 303 K. The obtained MOF particles are robust. The procedure has more impact on the crystalline and textural properties of MIL-53(Al) than on those of ZIF-8. The shaping procedure also has minor impact on the CO_2 adsorption capacity of the ZIF-8 while the MIL-53(Al) granules yielded higher CO_2 adsorption capacity losses: up to 24% at 15 bar of CO_2 pressure. The method employed in this work proves to be a viable and straightforward alternative for the preparation of ZIF-8 and MIL-53(Al) particles to be applied in gas-phase separation

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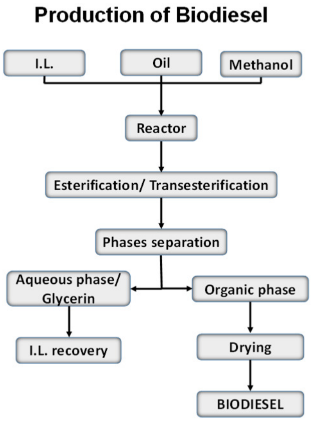
[P-RS28]

Production and characterization of biodiesel obtained by transesterification catalysed by ionic liquids based on imidazolium

A. Baú[1,2], *G. Gonçalves*[2], *A. Ribeiro*[1], *A. Queiroz*[1], *P. Brito*[1,*]
[1]*Mountain Research Center (CIMO), Polytechnic Institute of Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal;* [2] *Federal Technological University of Paraná, Campus Ponta Grossa, 84016-210 Ponta Grossa, Paraná, Brasil.*
** paulo@ipb.pt*

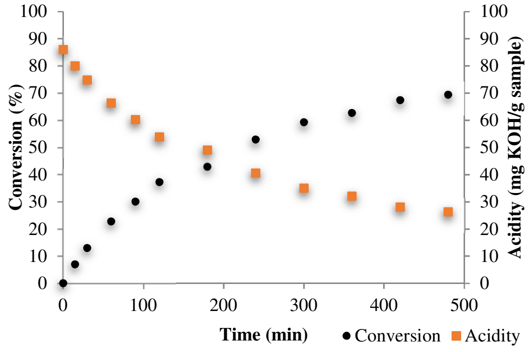


Biodiesel is a fuel that shows an increasing demand as a promising alternative to petroleum-based fuels. Biodiesel is produced by means of esterification or transesterification reactions, from renewable raw materials, as animal and vegetable oils and fats. The biodiesel generated by the traditional method of production proved that is economically and environmentally disadvantageous, due to this, in its production process changes are necessary to reduce its costs and make it an ecological product, such as, the introduction of used oils as feedstock. Moreover, the catalysts traditionally employed are not so effective due to the fact that these oils presents low quality, since they contain high levels of fatty acids in their composition. Ionic liquids arise as one promising solution to this problem, and some studies with hydrogen sulfate 1-butyl-3-methylimidazolium [BMIM][HSO_4] refer that this ionic liquid can be an viable catalyst choice for biodiesel production processes.

[P-RS29]

Esterification process catalyzed by ionic liquids for fatty acid methyl esters production

C. Meireles[1], *A. Queiroz*[1], *A. Ribeiro*[1], *P. Brito*[1,*]
[1]*Mountain Research Center (CIMO), Polytechnic Institute of Bragança, Campus Santa Apolónia, 5300-253 Bragança, Portugal.*
** paulo@ipb.pt*

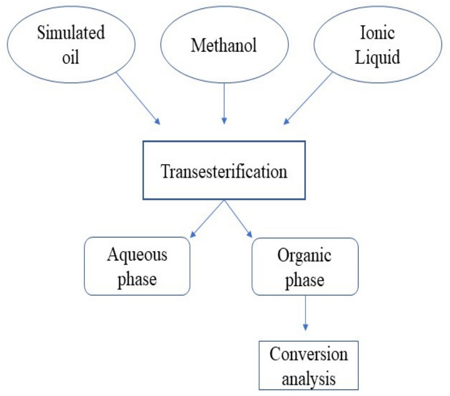


Due to the massive use of energy from non-renewable sources as well as to environmental problems it is important to find green alternatives. In this context the biodiesel production arises, as a possible diesel substitute which can be produced using basic or acid catalysts. Despite these traditional catalysts present high production yields, the problems that come from its use and the environmental impacts associated, result in the need for the search of more sustainable alternatives. The ionic liquids (IL) as possible catalysts represents an interesting alternative because IL are reusable and environmentally friendly. In present work, the main goal is to study biodiesel production using the ionic liquid 1-buthyl-3-methylimidazolium methyl sulfate [BMIM][MeSO$_4$] as catalyst, by the assessment of its kinetic activity. The results of kinetic study by the integral method, showed low activation energy of 5.16 kJ/mol and a pre-exponential factor (A) of 0.0624 $L^2.mol^{-2}.min^{-1}$.

[P-RS30]

Biodiesel production through transesterification applying ionic liquids as catalysts

H. Goes[1], *L. Lima*[2], *A. Queiroz*[1], *A. Ribeiro*[1], *P. Brito*[1*]
[1] *Mountain Research Center (CIMO), Polytechnic Institute of Bragança, Campus Santa Apolónia, 5300-253 Bragança, Portugal;*
[2]*Dept. of Chemical Engineering, Universidade Tecnológica Federal do Paraná, campus Londrina, Londrina-PR, Brasil.*
** paulo@ipb.pt*



The production of biodiesel started as an alternative and sustainable form of energy to reduce dependence on fossil fuels. This work aims to study the production by transesterification of biodiesel from simulated oil consisting of mixes of waste cooking oil and oleic acid, using as a catalyst ionic liquid (IL) 1-methylimidazolium hydrogen sulfate [HMIM][HSO$_4$]. The experimental tests were carried out using a two level total factorial design with one replicate, with three parameters: incorporated oleic acid (20% and 40% wt.), molar ratio oil/methanol (1:20 and 1:40) and reaction time (4h and 8h). The fixed operational conditions were: temperature (90ºC) and percentage of catalyst (10% wt.). The response studied was the conversion of the simulated oil. From the statistical analysis of the parameters, it was concluded that the parameters: reaction time and molar ratio oil/methanol, were those that showed the greatest influence on the result.

[P-RS31]

Phosphorus recovery from aqueous solutions with an eco-friendly adsorbent

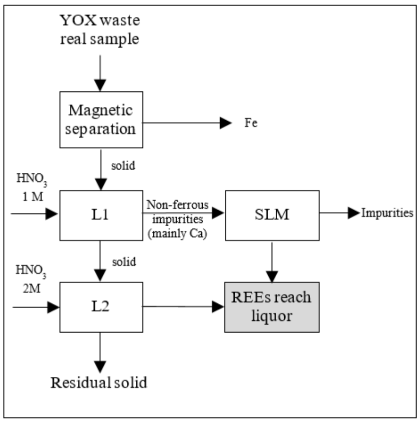
A.F. Santos[1], A. Arim[1,2], D.V. Lopes[1,3], L Gando-Ferreira[1], M.J. Quina[1,*]
[1] CIEPQPF, Chemical Process Engineering and Forest Products Research Centre. Department of Chemical Engineering, University of Coimbra, Portugal;[2] UNIPAMPA – Federal University of Pampa, Campus Bagé, Brazil; Avenida Maria Anunciaça˜o Gomes de Godoy, no. 1650, 96413-172 Bagé, Brazil; [3] CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal;
** guida@eq.uc.pt*

This work aims to evaluate the feasibility of recovery phosphorus by adsorption processes in batch and fixed-bed column, using thermal modified industrial waste (eggshell) as an adsorbent. The screening phase revealed that calcined eggshell at 700 ºC (CES700) is the best material. This adsorbent was characterized through nitrogen adsorption, XRD, SEM-EDS and thermogravimetric analysis. Through batch process, the influence of initial pH and adsorbent dosage were investigated. Langmuir-Freundlich model showed the best fitting to the equilibrium data, and the maximal adsorption capacity for CES700 was 39,0 mg P-PO_4/g. The kinetics of the process is controlled by a pseudo-first order model. Fixed-bed column experiments were conducted for studying the influence of most relevant operating conditions (feed concentration, superficial velocity). Yoon-Nelson, Thomas and Bohard-Adams models properly described the saturation curves, with values of R^2 equal or greater than 0.98.

[P-RS32]

REEs recovery from leach solutions of fluorescent lamp wastes using supported liquid membranes

S. Pavón[1,*], A.Fortuny[1], M.T. Coll[2], A.M. Sastre[3]
[1] Chemical Engineering Department, EPSEVG, Universitat Politècnica de Catalunya, Víctor Balaguer 1, 08800 Vilanova i la Geltrú, Spain; [2] Agri-Food Engineering and Biotechnology Department, ESAB, Universitat Politècnica de Catalunya, Esteve Terrades 8, 08860 Castelldefels, Spain; [3] Chemical Engineering Department, ETSEIB, Universitat Politècnica de Catalunya, Diagonal 647, 08028 Barcelona, Spain.
** sandra.pavon@upc.edu*

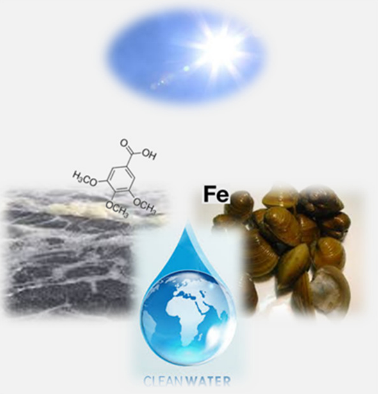


The quest for a circular economy developing green processes has swelled the interest on the end-of-life products processing. This paper proposes an alternative of the REEs recovery from leach solutions from fluorescent lamp wastes optimizing the leaching process and adding a SLM step. Red phosphor waste was undergone a first leaching to remove the main non-ferrous impurities (mainly Ca). Unfortunately, a small REEs amount was lost in this step. Thus, the leachate from L1 was treated in a SLM step using Cyanex 923 as a carrier. Nevertheless, when Na_2EDTA 0.05 M is used as receiving phase, the permeability coefficients were only linearly for low carrier concentrations (0.30-0.60 M) because a third phase is formed using high Cyanex 923 concentrations (0.90-1.20 M). This third phase can be avoided using a modifier such as the 2,6-dimethy-l-4-heptanone. Finally, the REEs recovery is possible with a second leaching step using HNO_3 or HCl 2 M.

[P-RS33]

Sludge free solar photo-Fenton combined with biofiltration for the degradation of phenolic compounds from olive mill wastewaters

E. Domingues[1], *J. Gomes*[1], *M. Gmurek*[1,2],*M.J. Quina*[1], *R.C. Martins*[1], *R.M. Quinta-Ferreira*[1]
[1]*CIEPQPF – Chemical Engineering Processes and Forest Products Research Center, Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, Pólo II – RuaSílvio Lima, 3030-790 Coimbra, Portugal;* [2]*Faculty of Process and Environmental Engineering, Department of Bioprocess Engineering, Lodz University of Technology, Lodz, Poland;*
**evadomingues@eq.uc.pt.*

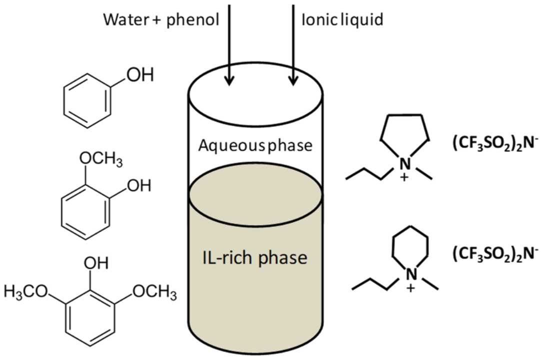


Fenton's process is an interesting wastewater treatment, while its main drawback is the dissolved iron remaining after the treatment that must be removed before releasingthe effluent. This generally leads to the production of iron sludge that constitutes a second source of pollution. The aim of this work is to study the efficiency of solar photo-Fenton on the degradation of olive mill wastewater. The use of light reduces the iron loads required for the reaction. In addition, the research also aims to infer about the possibility of combining solar photo-Fenton's with biofiltration using as hosts *Corbicula fluminea* to remove the iron remaining after treatment. This is an invasive species with high biofiltration capacity and tolerance to toxic compounds that can have an important role on wastewater treatment. Thus, an environmental application will be given to an alien species combining effluents depuration with pest management strategies.

[P-RS34]

Ionic liquids as solvent for the extraction of phenols from effluents of biomass fast pyrolisis

*E. J. González**, *I. Díaz, M. Rodríguez, M. González-Miquel, M. Hernández-Caricol*
Departamento de Ingeniería Química Industrial y del medioambiente, Universidad Politécnica de Madrid, C/José Gutiérrez Abascal, 2, E-28006 Madrid, Spain;
** ej.gonzalez@upm.es*

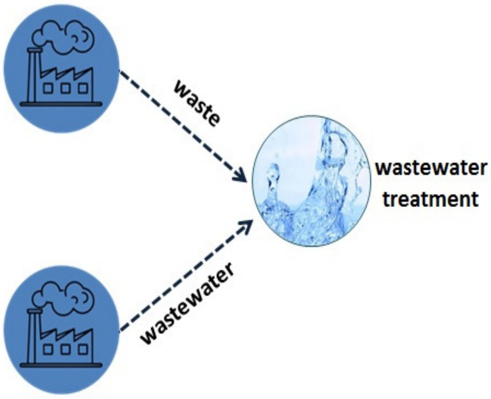


The goal of this work is to analyze the ability of 2 ionic liquids (ILs) as solvents to extract phenols from the aqueous fraction obtained after water washing of the oil generated in the fast pyrolysis of the biomass. This aqueous phase contains sugars that can be fermented to obtain bioethanol but also has phenols that must be removed before fermentation to prevent any damage to the microorganisms. In this work, the extraction efficiency of phenolic compounds using ILs as solvent is proposed as an alternative to the use of volatile organic compounds. This work was performed through equilibrium distribution studies. The phenol concentration was determined by absorbance measurements. The effects of phenol initial concentration and the chemical structure of phenols and ILs on the extraction process were analyzed and discussed. In all cases, high extraction efficiencies were obtained which has demonstrated the ability of these ILs to remove the phenolic compounds in this kind of streams.

[P-RS35]

Heterogeneous solar photo-Fenton using red-mud as low cost catalyst for olive mill wastewater treatment

E. Domingues[1], D.V. Lopes[1,2],J.R.Frade[2], M. Gmurek[1,3] ,M..J. Quina[1], R. C. Martins[1], , R. M. Quinta-Ferreira[1]
[1]CIEPQPF – Chemical Engineering Processes and Forest Products Research Center, Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, Pólo II – RuaSílvio Lima, 3030-790 Coimbra, Portugal, Portugal; [2]CICECO –Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro Portugal. [3]Faculty of Process and Environmental Engineering, Department of Bioprocess Engineering, Lodz University of Technology, Lodz, Poland;
** evadomingues@eq.uc.pt.*

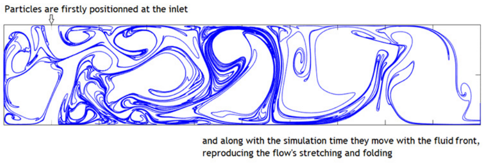


Red mud (a waste from the Bayer process) is an iron-rich material. The aim of the present research was to test it as a low-cost heterogeneous catalyst for dark and photo-Fenton's reaction on the abatement of the pollutant character of olive mill wastewater. Red mud showed low efficiency regarding the pollutants adsorption. However, the use of visible light was able to promote the photocatalytic oxidation of the phenolic acids tested. Moreover, the use of simulated visible light was able to truly improve Fenton's efficiency. In fact, the improvement was even higher than the one observed when Sun was applied as light source. In addition, low iron leaching was observed after the treatment processes. Red mud seems to be an interesting low-cost catalyst for heterogeneous photo-Fenton avoiding the production of iron sludges after the treatment. This work successfully combines waste management with wastewater treatment.

[P-RS36]

Lagrangian mixing simulation and quantification of scales

*J. Matos[1], M.S.C.A. Brito[1], M.M. Dias[1], J.C.B. Lopes[1], R.J. Santos[1]**
[1] Associate Laboratory LSRE-LCM, Faculdade de Engenharia da Universidade do Porto, Rua do Dr. Roberto Frias, 4200-465 Porto, Portugal.
**rsantos@fe.up.pt*



Lagrangian Mixing Simulation (LMS) is a new method that uses particles to track the mixing of two fluids. The line formed by the particles enables the calculation of interfacial area generation and the prediction of segregation scales. LMS is applied over 2D CFD simulation in a Confined Impinging Jets (CIJ) reactor for Re=100, 300 and 500. LMS shows that interfacial area generation is exponential for chaotic flows (Re=300 and 500) and linear for steady flows (Re=100). LMS is able to compute mixing scales smaller than 10^{-8} m, using desktop computers.

[P-RS37]

Modeling of carbonation and calcination reactions of Ca-looping process for CO_2 post-combustion capture in gPROMS®

M. A. Torres[1,2*], *P. Teixeira*[1,2], *R.M. Filipe*[3,4], *C.I.C. Pinheiro*[1,2], *H.A. Matos*[1,4]
[1] *Instituto Superior Técnico, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal;*[2]*Centro de Química Estrutural, Instituto Superior Técnico, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal;*[3]*Instituto Superior de Engenharia de Lisboa, R. Conselheiro Emídio Navarro 1, 1959-007 Lisboa, Portugal;*[4] *Centro de Recursos Naturais e Ambiente (CERENA), Instituto Superior Técnico, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal;*
** miguel.n.torres@ist.utl.pt*

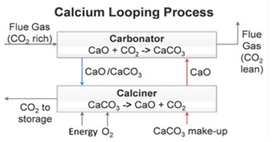


Figure 1. Schematic of Calcium Looping Process

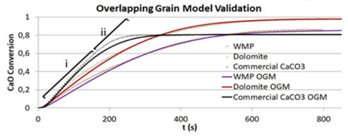


Figure 2. OGM validation for different sorbents. For Dolomite: i – Kinetic Regime, ii – Diffusional Regime;

In this work, the Overlapping Grain Model (OGM) [3] and A rate equation theory for the pore size distribution of calcined $CaCO_3$ (RThPSD) [4] were implemented in gPROMS® software. The OGM models the carbonation of CaO and the RThPSD the calcination of $CaCO_3$ and respective pore dynamics. The OGM was validated using data from fluidized bed reactor experiments, and accurately models the reaction regimes observed. The pore structure of the $CaCO_3$ particle was added as an initial condition to the RThPSD, and the calculation of surface area of vacancies was changed to avoid overestimating total pore area. The vacancy balance equation was also corrected to avoid undue pore volume disappearance. This work lays the basis for the simulation of sorbent deactivation in Ca-Looping by integration of both models, to be done after the validation

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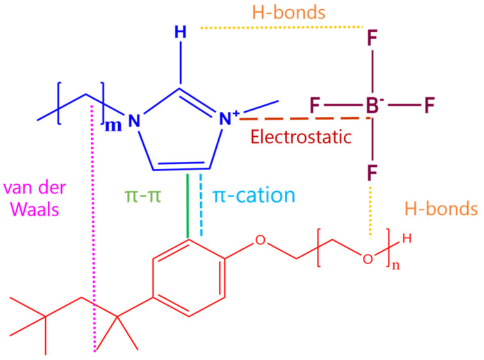
[P-RS38]

Modulating behavior of ionic liquid on micellization behavior in aqueous surfactant

I. Khan[1,2*], *M.A. Usmani*[3], *J.A.P. Coutinho*[2]
[1] *Department of Chemistry, Sultan Qaboos University, Box 36, Al-Khod 123, Oman;* [2] *CICECO - Aveiro Institute of Materials, Chemistry Department, University of Aveiro, 3810-193 Aveiro, Portugal;* [3] *Department of Chemistry Faiz-E-Aam College, Shahjahanpur, India.*
* *imran.pchr@gmail.com*, *imrank@squ.edu.om*

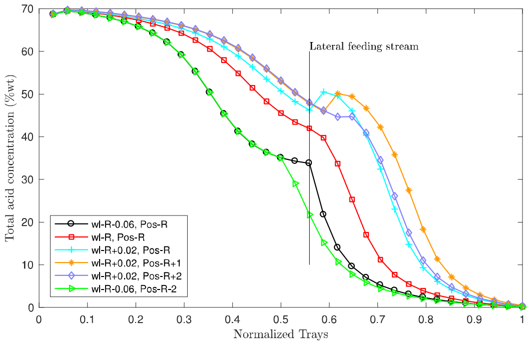


The intermicellar interaction study is of a great importance regarding its fundamental effect on micellar stability, which affects applied aspects of surface activity and micellar aggregation. Generally, the overall behavior of Ionic liquids (ILs) toward surfactants is determined by their electrostatic and hydrophobic interactions that are controlled by the structural properties of IL molecules including head group and counterion type and hydrophobic chain length. Besides, some ionic liquids are well-known for forming hydrogen bonding with water as well as with counterions and this can also influence ILs interaction with surfactants considerably and make it even more complicated. Thus, it is so difficult to generalize and predict about the effect of ILs on interfacial and aggregation properties of surfactants and any IL/surfactant mixture needs separate study as a specific case. To overcome this complexity, this review briefs the effect of IL with different chain lengths, cation and anion types on the surface activity, self-aggregation behavior, and aggregate morphology of cationic, anionic, zwitterionic and gemini surfactants in aqueous solution. Further, a comparative overview of all effects including ionic strength, temperature, electrolyte conditions such as salts and ionic liquids on intermicellar interaction has been discussed in terms of hydration, hydrophobic, and steric interactions on micellar stability.

[P-RS39]

Rigorous modelling of the NO_x absorption process: steady state sensitivity and validation of the dynamic behavior

I.L.S.B. Vilarinho[1,2,*], *N.M.C. Oliveira*[1], *B.P.M. Duarte*[1,3], *S.E.F.M. Pereira*[2]
[1] *CIEPQPF, Dept. of Chemical Engineering, Universidade de Coimbra, Rua Sílvio Lima – Pólo II, 3030-790 Coimbra, Portugal;* [2] *Bondalti, Quinta da Indústria – Rua do Amoníaco Português, 10, Beduído, 3860-680 Estarreja, Portugal;* [3] *Department of Chemical and Biological Engineering, ISEC, Polytechnic Institute of Coimbra, Rua Pedro Nunes, 3030-199 Coimbra, Portugal;*
**inessvilarinho@gmail.com*

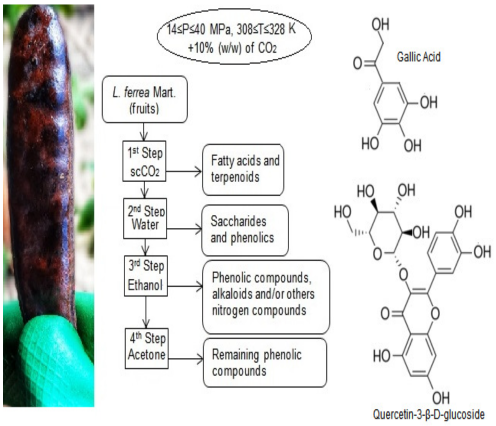


The absorption of nitrous oxides in nitric acid plants is a current industrial challenge due to stricter emission constraints and more demanding regulations, expected in a near future. To cope with this, the optimization of NO_x absorption systems is required. Here we describe the behavior of an industrial NO_x absorption column, using a simulation based strategy relying on a detailed mechanistic model. To demonstrate the usefulness of this tool, a sensitivity analysis of the steady state operation relative to changes in a diluted feed stream are considered. Next, the model is extended to simulate the dynamic behavior of the unit, and the simulation results are compared with industrial data. This tool evidences potential use both for dynamic optimization and control to reduce the NO_x emissions, as well as for process design and troubleshooting of existing industrial units.

[P-RS40]

Sequential extraction of phenolic compounds from *Libidibia ferrea* fruits using pressurized fluids

J. R. S. Botelho[1], *R.N.C. Júnior*[2], *H.C. de Sousa*[1*], *M.E.M. Braga*[1*]
[1] *CIEPQPF, Department of Chemical Engineering, FCTUC, University of Coimbra, Rua Sílvio Lima, Pólo II – Pinhal de Marrocos, 3030-790 Coimbra, Portugal;* [2]*LABEX (Laboratory of Extraction), Faculty of Food Engineering, Federal University of Pará, Rua Augusto Corrêa S/N, Guamá 66075-900, Belém, Pará,Brazil.*
**hsousa@eq.uc.pt; *marabraga@eq.uc.pt.*

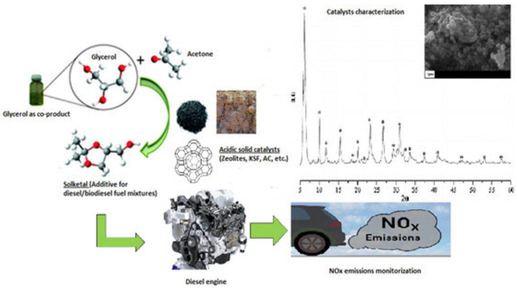


The phenolic compounds present in *Libidibia ferrea* (jucá) extracts are recognized to be responsible for the well-known biological activities. In this work, different pressurized fluids were sequentially employed for the fractionated extraction of jucá fruits. Supercritical carbon dioxide ($scCO_2$), water, ethanol and acetone were employed in the subsequent and sequential extraction steps. Results showed that extracts rich in fatty acids, phytosterols, lupeol and lupenone, were mainly obtained at the first $scCO_2$ extraction step, while pressurized acetone/CO_2 extractions were more selective for gallic acid and quercetin-3-β-D-glucoside. Obtained extract compositions are justified by the complex effects that operational temperature/pressure have on the relevant thermophysical properties that are known to affect solvent-based extraction methods, as well as by the raw material properties and chemical compositions after each extraction step that was performed.

[P-RS41]

Solketal, a fuel additive produced from the valorization of glycerol

J. Martinho[1,*], *J.Puna*[1,2], *M. T. Santos*[1], *H. T. Avelino*[1], *T. Trindade*[1], *J.M. Costa*[1]
[1] *Instituto Superior de Engenharia de Lisboa, R. Conselheiro Emídio Navarro, 1, Lisboa, 1959-007, Portugal;* [2] *CERENA, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1, Lisboa, 1049-001, Portugal.*
**a40620@alunos.isel.pt.*



Considering heterogeneous catalysts applied for the valorisation of glycerol, especially through its acetalization/acetylation reactions, several solid silica-alumina catalysts, like zeolites or natural clays (e.g. montmorillonites), seems to be very active catalysts in these processes, because they are cheap, non-corrosive, economically benign, with micro porosity and with high surface area and, easy to handle. Heterogeneous catalysis shows the typical processual advantages, when compared with the traditional homogeneous catalysts.In the present work, montmorillonite MMK10 with an atomic ratio of Si/Al = 10 obtained from natural sources, was activated to increase their acidity, to enhance its activity in the production of a fuel additive in diesel engines, like Solketal, an acetal obtained from the reaction of glycerol with acetone. This catalyst was characterised by SEM-EDS, FTIR and other structural and textural characterisation techniques. Catalytic tests of MMK10 were applied to produce Solketal, optimizing the several operating conditions, like temperature, reaction time, molar ratio of acetone/glycerol/ethanol (ethanol as co-solvent) and, the weight percentage of catalyst related with glycerol, the main raw-material in

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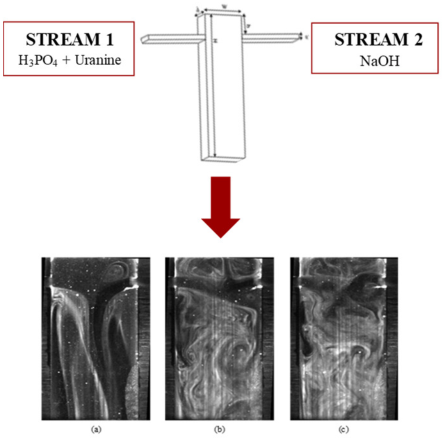
[P-RS42]

Reactive LIF test reaction for micromixing studies: definition of suitable operational conditions and validation in a T-jets mixer

J.P. Ribeiro[1,*], *M. Brito*[2], *L. Esteves*[2], *RJ. Santos*[2], *M.I. Nunes*[1]
[1] *CESAM - Centre for Environmental and Marine Studies/Department of Environment and Planning, University of Aveiro, Campus Universitário de Santiago 3810-193, Aveiro, Portugal;* [2] *Laboratory of Separation and Reaction Engineering, Universidade do Porto, Faculdade de Engenharia, Porto, Portuga.*
** joaoperes@ua.pt*

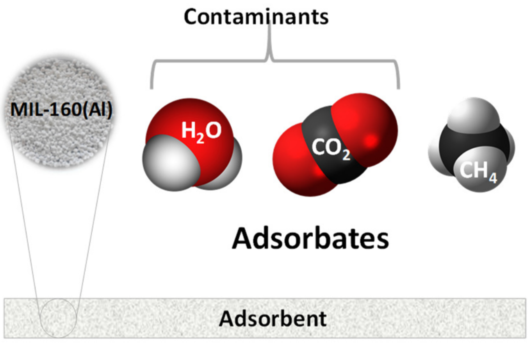


This work aimed to test and optimize one reactive PLIF method for (micro)mixing studies, consisting on an acid-base reaction with uranine as reactive tracer. The test-reaction was studied in a stopped-flow equipment to define suitable operational conditions, namely: chemical composition of the inflow streams to mix, concentration of reagents and fluorophore, excitation light wavelength and degradation of the streams (over a 24h-period) in increasing viscosity media. The most suitable operational conditions were tested in a T-jets mixer, illuminated in the axial plane with a laser light sheet, enabling to obtain fluorescence images inside this mixer. After adapting some of the operational conditions originally suggested in the literature, the test reaction became easier and suitable to be used in micromixing studies. Experiments performed in the T-jets mixer validated those operational conditions, showing the usefulness of this test reaction for micromixing studies.

[P-RS43]

CO_2 and CH_4 adsorption on MIL-160(Al) from dry and wet streams

M. P. Silva[1,], A.M. Ribeiro[1], C.G. Silva[1], U.-H. Lee[2], J. Faria[1], J. Loureiro[1], J.-S. Chang[2], A.E. Rodrigues[1], A. Ferreira[1]*
[1] Associate Laboratory LSRE-LCM, Department of Chemical Engineering Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, Porto, Portugal; [2] Institution Catalysis Center for Nanocatalysts, Korea Research Institute of Chemical Technology, Jang-dong 100, Yuseong Daejeon, Korea;
** mpsilva@fe.up.pt*

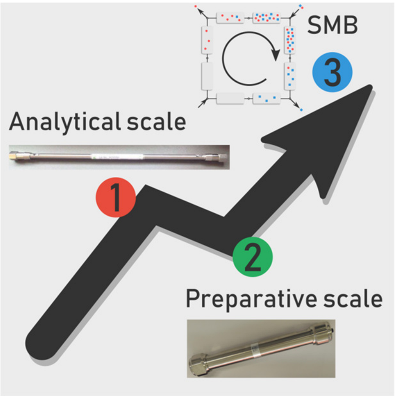


The presence of contaminants in natural gas/biogas leads to a reduction of heat value. Adsorption is one of the technologies used to upgrade the natural gas and the biogas, by removing the carbon dioxide (CO_2). In this study, the adsorption properties of different adsorbates, such as CO_2, methane (CH_4), and water (H_2O), on MIL-160(Al), were measured at three different temperatures. CO_2 and CH_4 adsorption equilibrium isotherms are of Type I. While the adsorption of water presents a Type IV shape. The dynamic experiments performed in a fixed-bed set-up included single component (CO_2, CH_4, and H_2O) adsorption and desorption experiments, in a bed initially filled with helium, as well as co-adsorption of CO_2 (or CH_4) with H_2O. Adsorption and desorption of CO_2 in a bed initially saturated with H_2O at 50% relative humidity was also studied. The breakthrough curves of CO_2 and CH_4 present a compressive front during the adsorption branch, and then a dispersive front during the desorption branch.

[P-RS44]

Study of triterpenic acids isolation by simulated moving bed at two distinct scales

J.P.S. Aniceto[1], I.S. Azenha[1], A. Mendes[2], C.M. Silva[1]*
[1] CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193, Aveiro, Portugal; [2] LEPABE - Faculdade de Engenharia, Universidade do Porto, 4200-465 Porto, Portugal.
** carlos.manuel@ua.pt*

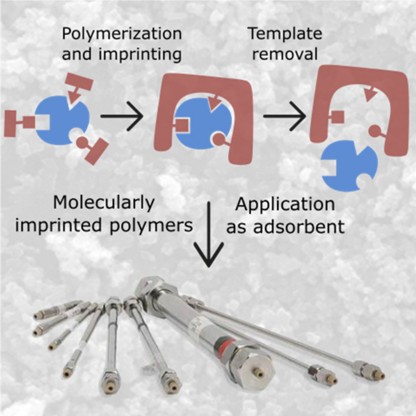


In this work the chromatographic separation of betulinic, oleanolic and ursolic acids (naturally occurring triterpenic acids with relevant bioactive properties) was studied at both analytical and preparative scales with the objective of implementing their separation by simulated moving bed (SMB). Preliminary HPLC experiments were conducted to select appropriate mobile and stationary phases. Equilibrium and mass transport parameters were determined through breakthrough experiments with pure compounds in a single analytical column. This information was then applied in the modeling of ternary breakthrough experiments conducted both at analytical and preparative scales. Finally, the SMB separation of the three compounds was simulated using a phenomenological rigorous model and applying data from analytical and preparative scale experiments, comparing the obtained results.

[P-RS45]

Molecularly Imprinted Polymers for the chromatographic separation of triterpenic acids isomers

J. P. S. Aniceto[1], *A. Rudnitskaya* [2], *C. M. Silva*[1*]
[1] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193, Aveiro, Portugal;*[2] *CESAM and Department of Chemistry, University of Aveiro, 3810-193, Aveiro, Portugal.*
* *carlos.manuel@ua.pt*

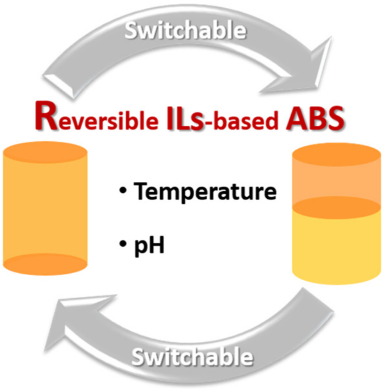


Molecularly imprinted polymers (MIPs) have been applied in many fields including in liquid chromatography as the stationary phase. These polymers are synthesized to possess binding sites highly selective to a given analyte, making them very promising sorbents especially for difficult separations in terms of selectivity. In this work, MIPs were developed with the purpose of being applied to the chromatographic isolation of betulinic, oleanolic, and ursolic acids, three triterpenic acids with significant pharmaceutical interest. Several MIPs were synthesized by thermal precipitation polymerization using oleanolic acid as template molecule, and different functional monomers and solvents. MIPs were analyzed by scanning electron microscopy and their adsorption ability towards the triterpenic acids was evaluated by batch adsorption experiments. A successful MIP was achieved which appears to exhibit infinite selectivity towards oleanolic acid.

[P-RS46]

Development of integrated processes applying reversible aqueous biphasic systems

A.M. Ferreira,[1] *H. Passos,* [1]*J.A.P. Coutinho*[1]*, M.G. Freire*[1*]
[1]*CICECO – Aveiro Institute of Materials, Chemistry Department, University of Aveiro, Portugal*
**maragfreire@ua.pt*



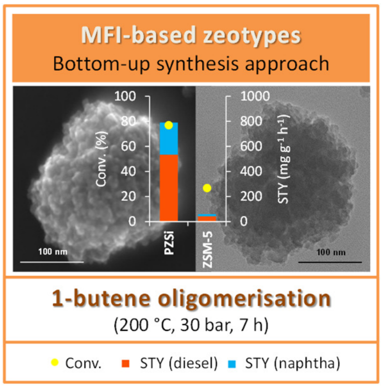
The ability to induce reversible phase transitions, e.g. between homogeneous solutions and biphasic liquid-liquid systems, is of paramount relevance in the development of integrated separation processes. Both pH- and temperature-triggered aqueous biphasic systems (ABS) composed of ionic liquids (ILs) are here disclosed as switchable liquid-liquid systems, and their application as integrated separation platforms is demonstrated.

[P-RS47]

Production of clean synthetic fuels using nanocrystalline MFI-based micro/mesoporous zeotypes synthesised *via* bottom-up approaches

A.F. Silva[1,*], *A.Fernandes*[2], *M.M. Antunes*[1], *M.F. Ribeiro*[2], *C.M. Silva*[1], *A.A. Valente*[1]

[1] *CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro, Portugal;* [2] *Institute for Biotechnology and Bioengineering, Centre for Biological and Chemical Engineering, Instituto Superior Técnico, Lisbon, Portugal.*
* *andreiafreitas@ua.pt*



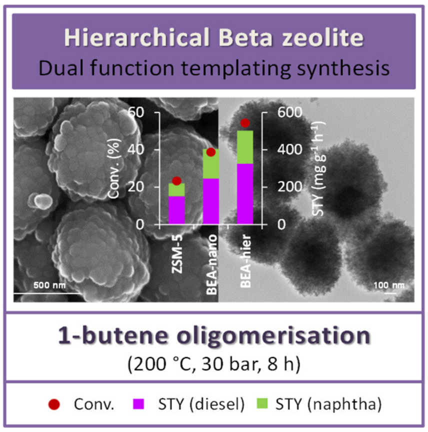
The oligomerisation of 1-butene was studied under high-pressure and continuous-flow operation (200-250 ºC, 30-40 bar), in the presence of micro/mesoporous zeotypes based on the MFI topology, prepared via different non-destructive bottom-up strategies, which influenced the material properties (morphology, textural and acid properties) and consequently the catalytic performances. In general, the zeotypes outperformed commercial zeolite ZSM-5, typically used in commercial oligomerization processes. The best-performing zeotype led to 77% conversion at 200 ºC and 30 bar.

[P-RS48]

Micro/mesostructured catalysts based on the BEA topology for 1-butene oligomerisation

A.F. Silva[1], *A. Fernandes*[2], *P. Neves*[1], *M.M. Antunes*[1], *S.M. Rocha*[3], *M.F. Ribeiro*[2], *C.M. Silva*[1], *A.A. Valente*[1,*]

[1] *CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro, Portugal;* [2] *Institute for Biotechnology and Bioengineering, Centre for Biological and Chemical Engineering, Instituto Superior Técnico, Lisbon, Portugal;*[3] *Department of Chemistry, QOPNA, University of Aveiro, Aveiro, Portugal.*
* *atav@ua.pt*

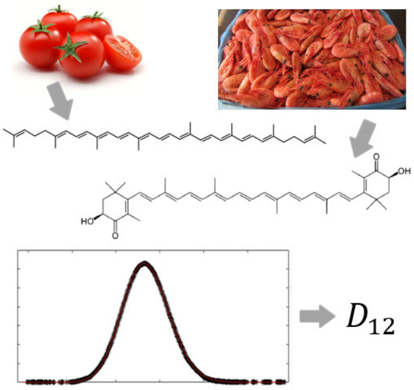


Mesostructured solid acid catalysts based on the BEA topology were explored for olefin oligomerisation, which is an attractive synthetic route to produce clean, sulphur-free fuels with reduced aromatics content. Specifically, the oligomerisation of 1-butene, which may derive from renewable sources, was carried out under high pressure and continuous-flow operation. The mesostructured catalysts consisted of a hierarchical zeotype (BEA-hier) synthesized *via* one-pot approach using a dual function template, and a composite (BEA/TUD) possessing zeolite nanocrystallites embedded in a mesoporous matrix synthesized under hydrothermal conditions. The influence of the material properties, catalyst activation temperature, and reaction conditions (pressure and temperature) were investigated, combining materials characterization, GC×GC-ToFMS and catalytic studies. The catalytic performances were compared to commercial nano- and microcrystalline zeolites possessing different topologies.

[P-RS49]

Measurement of diffusion coefficients of lycopene and astaxanthin in compressed liquids

J.M. Silva, B. Zêzere, I. Portugal, C.M. Silva, *
CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.
** carlos.manuel@ua.pt*



Lycopene and astaxanthin are two compounds with interest to the chemical, food and pharmaceutical industry due to their bioactive properties. The design and optimization of their industrial extraction and purification require equilibrium and kinetic data. Hence, in this work, their diffusion coefficients at infinite dilution were measured using the chromatographic peak broadening technique in the range 1-100 bar and 303.15-333.15 K. The solvents used were ethanol and ethyl acetate. The obtained diffusivities ranged from 3.447×10^{-6} to 6.679×10^{-6} cm^2 s^{-1} in the case of lycopene, and from 8.172×10^{-6} to 1.218×10^{-5} cm^2 s^{-1} in the case of astaxanthin. These data were modeled using several predictive and correlation models, with relative deviations between 5.00 and 91.29 % (lycopene) and 3.94 and 79.38 % (astaxanthin).

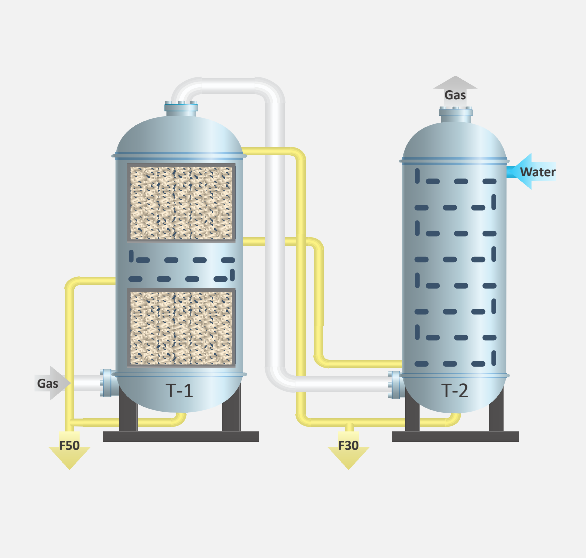
[P-RS50]

Model of a Formaldehyde Absorption System

C.G. Braz[1], *A. Mendes*[2], *J. Rocha*[3], *R. Alvim*[3], *Henrique A. Matos*[1,*],

[1] *Centro de Recursos Naturais e Ambiente, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal;* [2] *Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculdade de Engenharia, Universidade do Porto, R. Dr. Roberto Frias, 4200-464 Porto, Portugal;* [3] *EuroResinas – Indústrias Químicas S.A., Plataforma Industrial de Sines – Lote Industrial I, 7520-064 Sines, Portugal;*

** henrimatos@tecnico.ulisboa.pt.*



Formaldehyde is produced on a large scale due to its many applications as a raw material in industrial and end-use products. Because it is impossible to handle in its pure gaseous form, formaldehyde is almost entirely produced as an aqueous solution (formalin) by removing it from a gaseous stream in a system of absorption columns. Formalin is obtained with concentrations of around 55 and 35 w%.

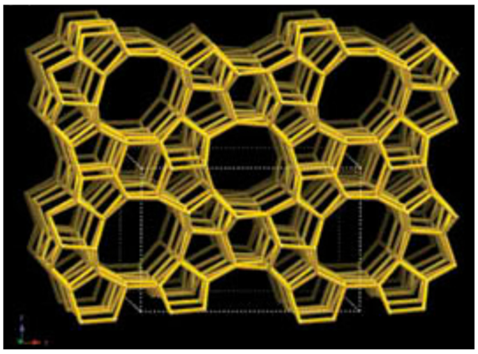
The absorption system studied involves a column (T-1) with two sections of random packing, with a section of trays in between, and a second column (T-2) with trays that include internal cooling coils. A non-equilibrium mass transfer model of the industrial absorption system was implemented in *gPROMS® Modelbuilder*. The model combines the multicomponent mass transfer phenomena with the reactions in the liquid phase.

The results are mainly in accordance with the plant data. The columns temperature and composition profiles generated by the model will be validated in future work.

[P-RS51]

Synthesis and characterisation of aluminosilicate ZSM-5 membranes

*S. Costa, S. P. Cardoso, Z. Lin, C. M. Silva***
CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;
** carlos.manuel@ua.pt*



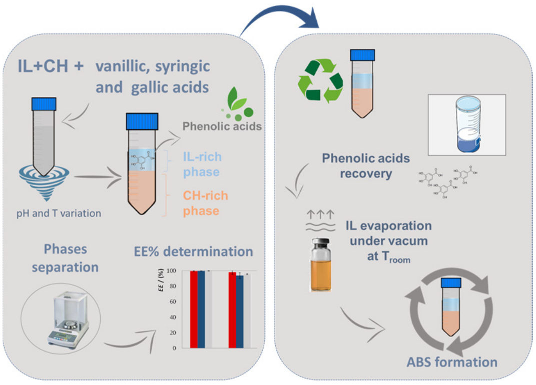
Aluminosilicate ZSM-5 membranes have been prepared on a tubular porous α-alumina support using a seeding by suspension method, followed by hydrothermal secondary growth synthesis. These membranes have been subsequently characterised by X-Ray Diffraction and Scanning Electron Microscopy. Permeation experiments have been performed under fixed and programmed temperature in the range of 298-383 K, using He, N_2 and O_2. The permeance results (expressed in mol m^{-2} s^{-1} Pa^{-1}) vary between 1.08×10^{-6} and 1.93×10^{-6} for He, from 1.04×10^{-7} to 2.20×10^{-7} for N_2, and between 5.69×10^{-8} and 1.36×10^{-7} for O_2. While the results for O_2 and N_2 are comparable with the ones found on the literature, the permeance of He is higher than expected. The quality of the membrane was proved, discarding the existence of macro and mesodeffects.

[P-RS52]

Ionic liquids and carbohydrates in aqueous media: Novel sustainable separation platforms

S.N. Pedro[1] *, M.V. Quental*[1]*, M.M. Pereira*[1]*, A.M. Ferreira*[1]*, S. Shahriari*[2]*, A. Mohamadou*[3]*, J.A.P. Coutinho*[1]*, M.G. Freire*[1]

[1]*CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;* [2]*Department of Chemical Engineering, Islamic Azad University, Shahr-e-Qods Branch, Tehran, Iran;* [3]*Université de Reims Champagne-Ardenne, Institut de Chimie Moléculaire de Reims (ICMR), CNRS UMR 7312, UFR des Sciences Exactes et Naturelles, Reims, France.*
soniapedro@ua.pt

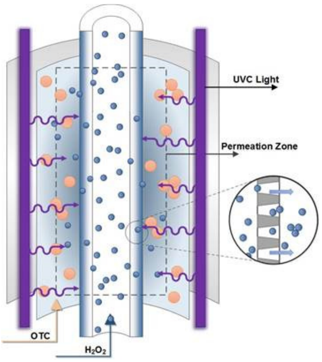


Ionic-liquid-based aqueous biphasic systems (IL-based ABS) represent an appealing alternative to the current separation and purification processes. To this end, imidazolium-based ILs and inorganic salts are commonly used as phase-forming components of ABS. Nevertheless, these compounds display some biodegradability and toxicity concerns, boosting the research on alternative ILs derived from natural sources. Aiming at establishing effective and sustainable processes, carbohydrates were combined with tetralkylphosphonium and tetralkylammonium-based ILs to form ABS. Their ability to form two-phase systems was evaluated by the determination of the respective phase diagrams, followed by the appraisal of their applicability as separation processes. These systems were tested for the separation of antioxidants at different temperatures and pH conditions. It was found that these novel systems are competitive separation platforms when compared to ABS formed by less biocompatible ILs and salts.

[P-RS53]

UVC coupled tube-in-tube membrane microreactor using on-demand H_2O_2 injection for oxytetracycline degradation

P. Alfonso-Muniozguren[1,], J.P. Monteiro[2], J. Lee[1], S.M. Miranda[2], R.A.R. Boaventura[2], V.J.P. Vilar[2]*
[1] Chemical and Process Engineering, University of Surrey, Guildford, United Kingdom; [2] Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (Associate Laboratory LSRE-LCM), Faculty of Engineering, University of Porto, Porto, Portugal.
**p.alfonso@surrey.ac.uk*

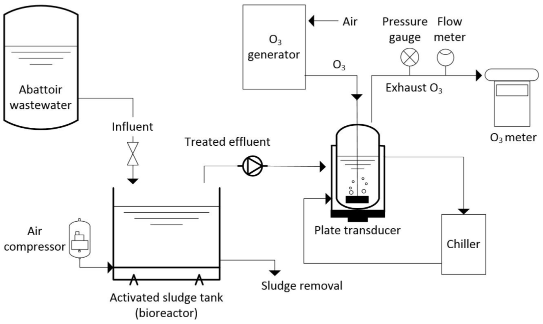


With the purpose of increasing the efficiency of UVC/H_2O_2 coupled systems for the treatment of contaminants of emerging concern, an innovative setup is proposed. The principle novelty of the new tube-in-tube membrane microreactor relies on the continuous, uniform and on-demand dosing of H_2O_2. An ultrafiltration membrane is used as a dosing system to deliver on demand H_2O_2 into the anulus of the reactor. In the anulus, where the liquid to be treated flows, UVC light is provided via four mercury lamps located externally to the outer tube. Keeping a constant gradient of the chemical across the whole length of the reactor, process efficiency could be increased, leading to a reduction in the use of the chemical, as well as a decrease in treatment time. Besides providing a better performance, the reactor has the advantage of an easy upscaling into a real plant.

[P-RS54]

Acoustic cavitation combined ozonation for real abattoir wastewater treatment

P. Alfonso-Muniozguren[1,], M.H. Bohari[1], C. Avignone-Rossa[2], A. Sicilia[2], M. Bussemaker[1], D. Saroj[3], J. Lee[1,*]*
[1]Chemical and Process Engineering, University of Surrey, Guildford, GU27XH; [2]Faculty of Health and Medical Sciences, Microbial Sciences, University of Surrey, Guildford, GU27XH; [3] Civil and Environmental Engineering, University of Surrey, Guildford, GU27XH.
** p.alfonso@surrey.ac.uk*

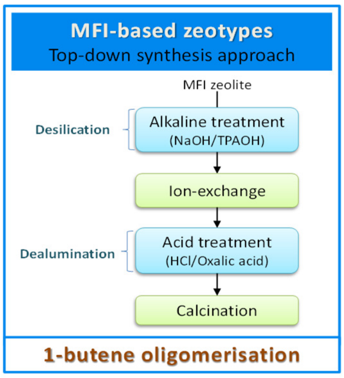


Wastewater pollution is becoming a worldwide concern due to new and tighter environmental regulations, and the increasing need for fresh water for the exponentially growing population. Therefore, suitable wastewater treatment methods are required to ensure the wastewater quality meet regulations before discharge. In the present study a combined lab scale ozonation-sonication system was used to treat an activated sludge effluent from a real abattoir, comparing the treatment efficiency of the processes. Ozone and ultrasound (separately and combined) were used as tertiary treatment methods, using different ultrasonic frequencies (44, 300 and 1000 kHz), applied sonication powers (10-40 W) and treatment times (1-60 min). Results were analysed for COD, BOD, total suspended solids, pH, total coliforms and total viable counts and compared to water discharge and reuse

[P-RS55]

Production of clean synthetic fuels using nanocrystalline MFI-based micro/mesoporous zeotypes synthesised *via* top-down approaches

A.F. Silva[1,*], *A. Fernandes*[2], *M.M. Antunes*[1], *M.F. Ribeiro*[2], *C.M. Silva*[1], *A.A. Valente*[1]
[1] *CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro, Portugal;* [2] *Institute for Biotechnology and Bioengineering, Centre for Biological and Chemical Engineering,* [3]*Instituto Superior Técnico, Lisbon, Portugal.*
** andreiafreitas@ua.pt*



The oligomerization of light olefins is an alternative route to produce synthetic clean fuels and other high added-value products. The oligomerisation of 1-butene was studied under high-pressure (30 bar) and continuous-flow operation, in the presence of micro/mesoporous zeotypes based on the MFI topology, prepared via different destructive top-down strategies, using a commercial ZSM-5 zeolite. The different approaches influenced the material properties and consequently the catalytic performances.

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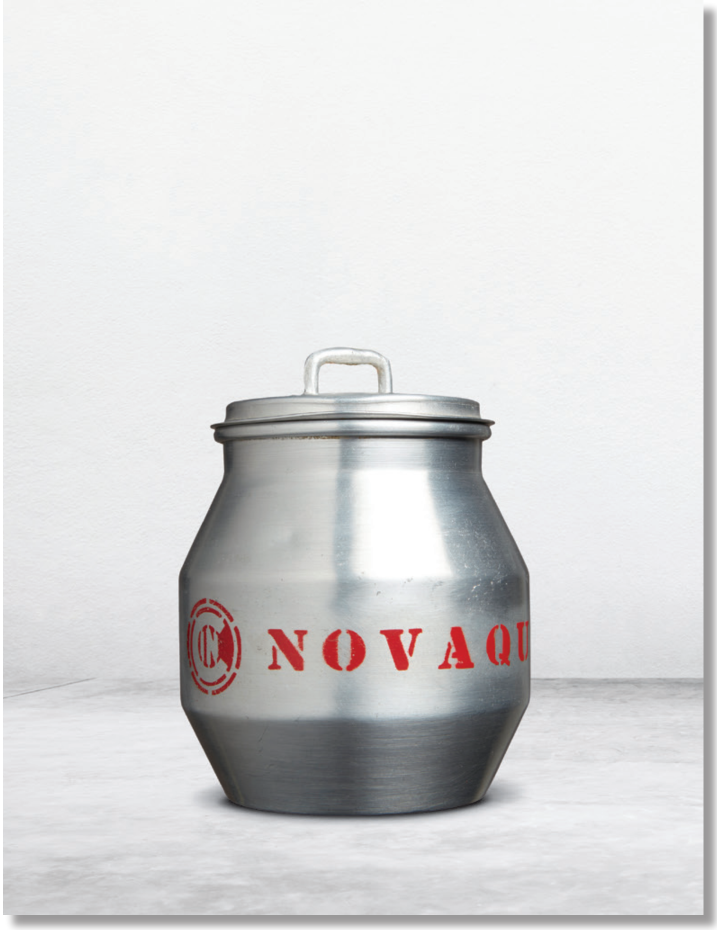

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PARA: MUNDO

Há 100 anos a fazer
as cores de Portugal.

Muita coisa mudou desde 1917 até hoje. E a CIN assistiu a tudo. Vimos todo um país e também o mundo mudarem. E a CIN também mudou. Em 100 anos passámos de uma fábrica no Porto a líder nacional e ibérica do mercado de tintas e vernizes. E se hoje celebramos um século é graças à sua preferência. Obrigado por dar cor também ao nosso mundo.

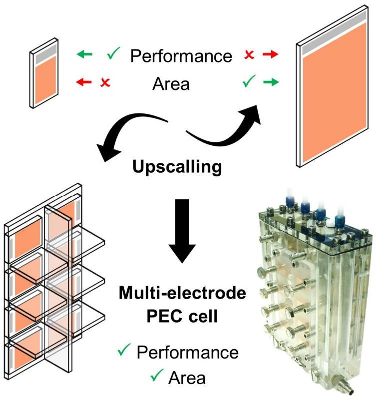
Poster Session

ENERGY AND ENVIRONMENT

[P-EE01]

Multi-electrode window for large-area solar hydrogen production

A. Vilanova[1], T. Lopes[1], A. Mendes[1, *]
[1] LEPABE - Faculdade de Engenharia, Universidade do Porto, rua Dr. Roberto Frias, 4200-465 Porto, Portugal.
* mendes@fe.up.pt

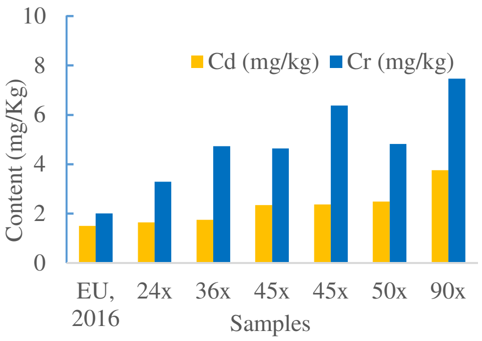


One of the main challenges in the field of photoelectrochemical water splitting is the difficulty of preparing high-performing photoelectrodes with a large active area. This work reports a multi-electrode window assembled in the CoolPEC cell for holding up to eight small photoelectrodes connected in parallel. Internal separators placed between electrodes avoid parasitic ionic paths and overpotential losses, as demonstrated with CFD simulations. Each separator is strategically perforated to preserve the main flow path lines inside the cell, avoiding the accumulation of evolved gas bubbles and assuring proper heat dissipation. *J-V* measurements show that neither the photocurrent density nor the photovoltage are affected when eight hematite photoelectrodes are operated in parallel; without internal separators a current loss of *ca.* 15 % is observed. The negative effect of an underperforming photoelectrode decreases exponentially with the number of photoelectrodes connected in parallel.

[P-EE02]

Investigation of the viability of converting a leachate from a mechanical biological treatment plant for municipal solid waste into fertilizers

J. Cardoso[1,*], B. Rodrigues[2], H. Gomes[1], P. Brito[1]
[1] Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-252 Bragança, Portugal; [2] Resíduos do Nordeste, EIM, Rua Fundação Calouste Gulbenkian, Mirandela, Portugal.
* jonathancardoso@ipb.pt

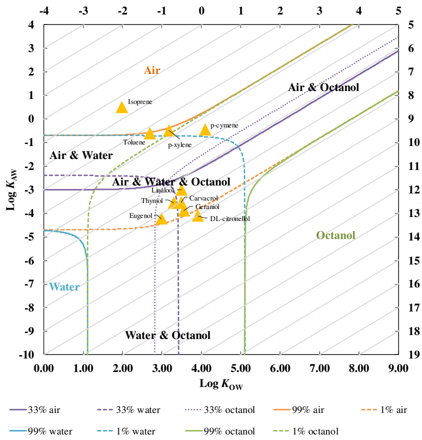


The main environmental issue associated with the compost production is the production of a liquid leachate. However, the leachate may also be considered as a source of nutrients and used as fertilizer. The main concern is loading the soil with metals that can result in increased metal content of crops. This work intends to determine the physical and chemical properties of a raw leachate from a mechanical biological treatment plant for municipal solid waste, to assess the possibility of converting it into as commercial fertilizer which meets to the specifications required in the proposal of regulation of the European Parliament of 2016, for fertilizers. In a preliminary study, it is concluded that the leachate qualitatively meets the requirements established for the composition of commercial fertilizers and the production cost of leachate as raw material is low.

[P-EE03]

Hydrophobic monoterpenes: myth or reality?

M.A.R. Martins[1-3,], L.P. Silva[1], J.A.P. Coutinho[1], S.P. Pinho[2,3,*]*
[1] CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal; [2] Associate Laboratory LSRE-LCM, IPB, 5300-253 Bragança, Portugal; [3] Mountain Research Center – CIMO, IPB, 5301-855 Bragança, Portugal;
**moniamartins@ua.pt ; spinho@ipb.pt*

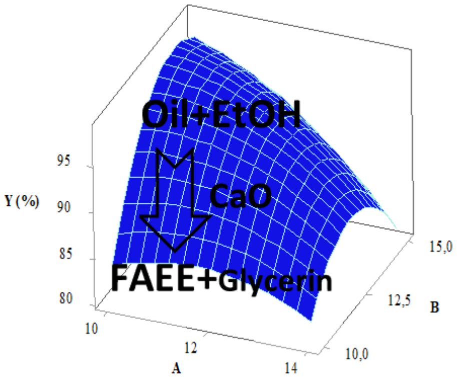


Terpenes belong to the largest and most diverse class of natural products. Due to the increasing importance of their applications and the emerging perception of their impact on the environment, the available physicochemical characterization is insufficient. In this work the solubility of terpenes in water at six different temperatures was evaluated. Due to the low solubility of these compounds a novel technique was adopted for their measurements and validated using the aqueous solubility data for sparingly soluble aromatic compounds. The experimental information is shown in a two-dimensional chemical space diagram providing indications to their probable distribution in the environment once released. This work contributes and calls for increasing the availability of reliable experimental property data of terpenes, which are also of enormous importance to the improvement, development and test new computational methods aiming for their prediction in such a vast family of compounds.

[P-EE04]

Optimization of soybean oil ethanolysis by response surface methodology

M. Ramos[1,2,], M. Catarino[2], A.P.S. Dias[2], J. Puna[1,2]*
[1] ISEL, Rua Conselheiro Emídio Navarro, 1, Lisboa, 1959-007 Portuga; [2] LAETA, IDMEC, CERENA, IST, Universidade de Lisboa, Av. Rovisco Pais, s/n, Lisboa, 1049-001 Portugal
**martasaramos@tecnico.ulisboa.pt*

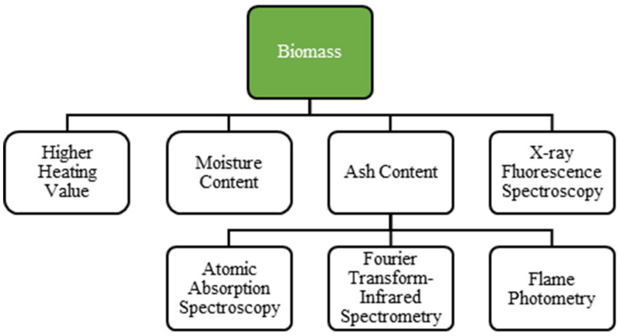


Biodiesel was successfully produced from soybean oil ethanolysis using a basic heterogeneous CaO catalyst. A green CaO catalyst was obtained by calcination of scallop shells (food waste). The heterogeneous catalyzed ethanolysis reaction conditions were optimized using a RSM methodology. The influence of reaction variables such as ethanol:oil molar ratio (10:1-14:1), catalyst loading (10-15 % based on oil weight) and time reaction (6-10 h) on the FAAE yield were analyzed. Computation was made using *Minitab* software. The optimal reaction parameters achieved were: 11:1 ethanol: oil molar ratio; 13.8 % catalyst loading and 9.1 h with 99.2 % maximum FAEE yield predicted. The fitted model was verified for the optimal conditions giving 99.0% of FAEE yield instead of the 99.2% predicted.

[P-EE05]

Preliminary analysis of ashes from different agricultural and forestry biomass residues

D. Marques[1], D. Direito[1], M. Reinhardt[2], A.F. Almeida[1], R.M. Pilão[1], A.M. Ribeiro[1]*
[1] CIETI, Instituto Superior de Engenharia do Porto (ISEP), Rua Dr. António Bernardino de Almeida, 431, 4200-072 Porto, Portugal;[2] Erasmus Student, Chemical Engineering Dept., ISEP, Rua Dr. António Bernardino de Almeida, 431, 4200-072 Porto, Portugal.
** asr@isep.ipp.pt*

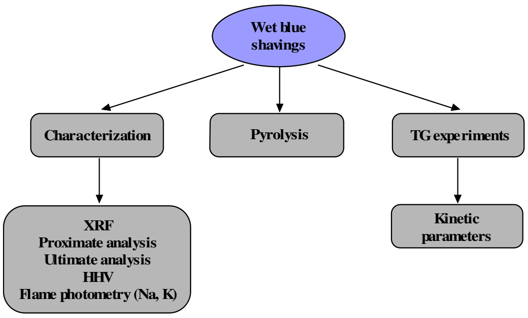


Six different lignocellulosic biomasses (hazelnut and almond shells, pine cones, pine bark, olive bagasse, and fine high-density cork granules) were characterized in terms of moisture, ash content, and higher heating value (HHV). X-ray fluorescence spectra of the various materials show traces of Ca, K, Si, Fe, Mn, P, Cl in the samples. After acid digestion, flame photometry was used to determine K and Na content in the ashes. Ca, Mg and Fe concentrations in the ashes were measured by atomic absorption spectrometry. The ashes were also characterized by Fourier transform infrared spectroscopy (FTIR) in the range 600 to 2300 cm^{-1}. Olive bagasse presented the highest ash content (5.8 %) and HHV (20.8 MJ/kg) values. Almond shell ash had the highest K and Na content (27.3 % and 26.3 %, respectively). Fine high-density cork granule ash contained the greatest Ca concentration (25.7 %), and pine bark ash had the highest Mg content (2.8 %). FTIR spectra showed the presence of Si in all ashes.

[P-EE06]

Thermochemical behaviour of wet blue shavings in an inert atmosphere

D. Direito[1], A.F. Almeida[1], R.M. Pilão[1], A.M. Ribeiro[1,3]
[1] CIETI, Instituto Superior de Engenharia do Porto (ISEP), Rua Dr. António Bernardino de Almeida, 431, 4200-072 Porto, Portugal.
** asr@isep.ipp.pt*

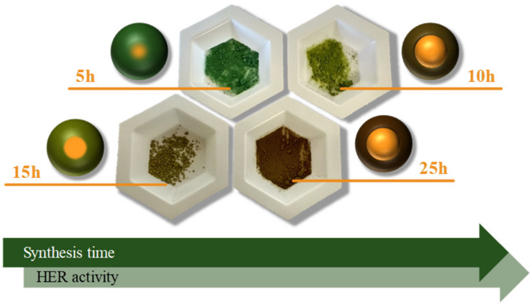


The main objective of this investigation was to study the thermal decomposition of wet blue shavings using two techniques: TG experiments (with the determination of kinetic parameters) and a slow pyrolysis experiment at a set temperature of 700 ºC and at a heating rate of 20 $ºC.min^{-1}$. The residues were characterized in terms of their ultimate and proximate analysis, chromium oxide content and higher heating value. The thermogravimetric experiments show that decomposition of the wet blue shavings occurs into two stages: the first corresponds to the drying of the material, the second is related to the thermal decomposition of the leather waste. The kinetic parameters of the second stage of decomposition were determined by applying the method of Coats-Redfern. For the pyrolysis experiment at a set temperature of 700 ºC and HR = 20 $ºC.min^{-1}$, the yield of the biochar obtained was 27.1%. The gas produced contained CO_2, CH_4, CO and H_2.

[P-EE07]

Influence of the synthesis conditions on the selectivity of CuZn catalysts towards CO_2 electrochemical reduction ($ERCO_2$)

*C. Azenha**, *C. Mateos-Pedrero, A. Mendes*
LEPABE - Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal
** catia.azenha@fe.up.pt*

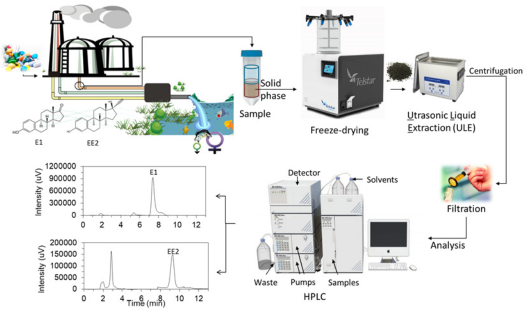


A series of CuZn catalysts were prepared through a solvothermal route using different synthesis time: 5 h, 10 h, 15 h and 25 h. The CuZn 5 h catalyst was the best performing catalyst with the highest selectivity towards electrochemical reduction of CO_2 ($ERCO_2$). CuZn 10 h achieved the highest overall current density (12.34 $mA{\cdot}cm^{-2}$, in CO_2-saturated electrolyte), however, with expressive contribution of the hydrogen evolution reaction (HER). The HER reaction is enhanced increasing the catalyst synthesis time.

[P-EE08]

Development of a simple and inexpensive methodology for the determination of estrone and 17α-ethinylestradiol in sludge samples

V. Louros[1,*], *D. Lima*[2,3], *J. H. Leitão*[4], *V. Esteves*[2], *H. Nadais*[1]
[1] *CESAM & Department of Environment and Planning, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal;* [2] *CESAM & Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal;* [3] *Instituto Politécnico de Coimbra, ESTESC-Coimbra Health School, Department of Complementary Sciences, Rua 5 de Outubro, S. Martinho do Bispo, 3046-854 Coimbra, Portugal;* [4] *iBB-Institute for Bioengineering and Biosciences, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal.*
** vitorialouros@ua.pt.*

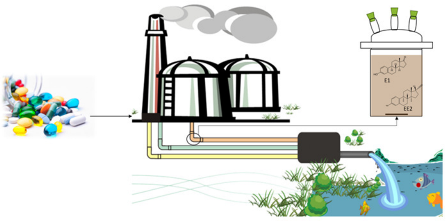


Estrone (E1) and 17α-ethinylestradiol (EE2) are becoming increasingly recognised as important micropollutants to be monitored in wastewater treatment plants (WWTPs). This study describes a method for the simultaneous determination of E1 and EE2 in fresh sludge samples. After spiking fresh digested sludge with E1 and EE2 standards and maintaining contact during 5, 30 and 60 min, the freeze-dried samples were subjected to ultrasonic liquid extraction (ULE), with methanol and acetone, and analysed by high-performance liquid chromatography with a fluorescence detector (HPLC-FLD). The recoveries obtained for E1 and EE2 were 103 ± 3% and 97 ± 4%, respectively. Fresh sludge samples from a WWTP located in Portugal were analysed and only E1 was detected at a concentration in the range of 1.00 - 4.8 $\mu g\ g^{-1}$. The method here developed is fast and simple, reliable and inexpensive, making possible its application for monitoring the contamination of sludge with these estrogens.

[P-EE09]

Removal of estrone and 17α-ethinylestradiol by digested sludge under different conditions using batch experiments

V. Louros[1,*], A. Sousa[2], D. Lima[3,4], J. H. Leitão[5], V. Esteves[3], H. Nadais[1]
[1] CESAM & Department of Environment and Planning, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal; [2] Department of Environment and Planning, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal; [3] CESAM & Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal; [4] Instituto Politécnico de Coimbra, ESTESC-Coimbra Health School, Department of Complementary Sciences, Rua 5 de Outubro, S. Martinho do Bispo, 3046-854 Coimbra, Portugal; [5] iBB-Institute for Bioengineering and Biosciences, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal.
** vitorialouros@ua.pt*

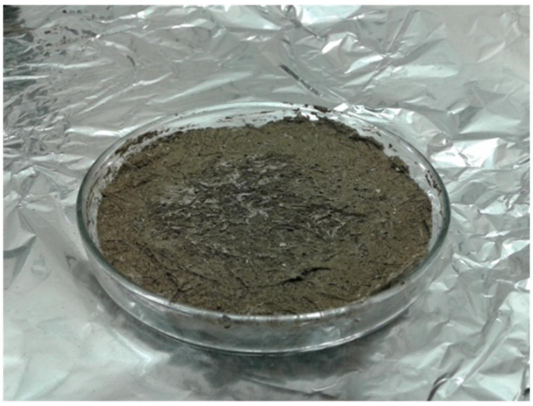


The natural estrogen estrone (E1), and the synthetic estrogen 17α-ethinylestradiol (EE2) are of great environmental concern. The adsorption and degradation of E1 and EE2 by activated sludge under anaerobic conditions were investigated by a series of batch experiments. Different treatment conditions were used, including three temperatures (20 °C, 25 °C and 34 °C), three mixed liquor suspended solid (MLSS) (2 g L^{-1}, 3 g L^{-1} and 5 g L^{-1}) and the addition of nitrate. E1 and EE2 were removed from the liquid phase in contact with activated sludge and the rapid adsorption of E1 and EE2 was observed. The E1 was degraded fastest by the bacterial community. On the other hand, EE2 tended to remain longer in sludge solid phase. Temperature seems to be the factor that most influenced the removal of E1 and EE2 from the sludge. In a biological reaction process, both adsorption and degradation processes may occur simultaneously, however, adsorption seems to be the dominant process.

[P-EE10]

Solid-liquid extraction for the determination of volatile methylsiloxanes (VMSs) in sewage sludge samples

J. Silva[1], F. Bernardo[1], N. Ratola[1], A. Alves[1], V. Homem[1,*]
[1] LEPABE – Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;
**vhomem@fe.up.pt*

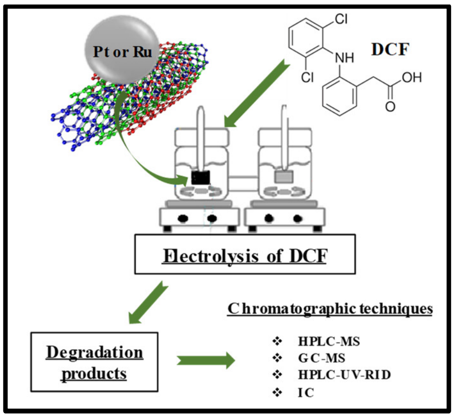


Volatile methylsiloxanes (VMSs) present low solubility and high octanol-water partition coefficients, tending to adsorb onto the extracellular polymeric substances (EPS) of the sewage sludge flocs, instead of accumulating in the water phase of the wastewater treatment plants (WWTPs). A method based on solid-liquid extraction followed by gas chromatography-mass spectrometry was successfully applied to detect and quantify seven VMSs (L3, L4, L5 and D3, D4, D5 and D6) on sewage sludge samples. The proposed methodology was validated, providing a good linearity range (5 to 1500 µg/L) and limits of detection (LODs) between 0.0004 (D5) and 0.47 (L3) ng/g dw. Considering this complex matrix, good precision (average relative standard deviation < 15%) and accuracy (recoveries of 69% for D3 to 124% for D5) were achieved. The method was successfully applied to analyze sludge samples collected in different WWTPs. Cyclic siloxanes were the predominant compounds (98%), especially D5.

[P-EE11]

Electrochemical degradation of Diclofenac on catalysts based on CNT and M/CNT modified electrodes

M. Ferreira[1], *S. Güney*[2], *I. Kuźniarska-Biernacka*[1], *O. S. G. P. Soares*[3], *M. F. R. Pereira*[3], *J. L. Figueiredo*[3], *I. C. Neves*[1,4], *A. M. Fonseca*[1,4], *P. Parpot*[1,4*]
[1] *CQUM, Center of Chemistry, University of Minho, 4710-057 Braga, Portugal;* [2] *Department of Chemistry, Technical University of Istanbul, Maslak, 34467 Sarıyer/İstanbul, Turkey;* [3] *Laboratory of Catalysis and Materials (LCM), Associate Laboratory LSRE-LCM, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Porto, Portugal;* [4] *CEB, Center of Biological Engineering, University of Minho, 4710-057 Braga, Portugal.*
* *contact_ parpot@quimica.uminho.pt*

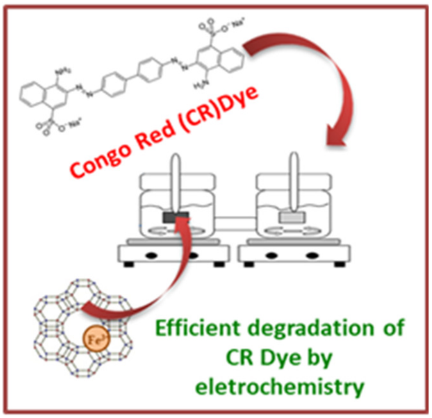


Diclofenac (DCF) - a nonsteroidal anti-inflammatory drug - is one of the most frequently detected pharmaceutical compounds in the aquatic environment. Because of its negative effects on public health and environment, this emerging pollutant monitoring and removal from wastewater are of high importance. Electrochemical oxidation has attracted growing interest in the last years, due to its versatility, high efficiency and environment compatibility.Electrochemical oxidation of DCF has been studied using multiwalled carbon nanotubes (CNT) and monometallic catalysts based on carbon nanotubes (M/CNT), at different pH media. The electroreactivity of DCF on modified electrodes and the kinetic parameters of the redox reactions were determined using cyclic voltammetry. Electrodegradation of DCF in aqueous medium was carried out using long-term electrolyses. The products of these electrolyses were identified and quantified by HPLC-MS, GC-MS, HPLC-UV-RID and IC.

[P-EE12]

Fe(III)NaY$_{nano}$ as efficient electrocatalyst for electrodegradation of Congo Red dye

Z. Bencheqroun[1,3], *M. Ferreira*[1], *H. Zaitan*[3], *M. Nawdali*[4], *A. M. Fonseca*[1,2], *P. Parpot*[1,2*], *I. C. Neves*[1,2]
[1] *CQUM, Center of Chemistry, University of Minho, Braga, 4710-057, Portugal;* [2] *CEB, Center of Biological Engineering, University of Minho, Braga, 4710-057, Portugal;* [3] *Laboratoire de Chimie de la Matière Condensée, Faculté des Sciences et Techniques, Fès- Maroc;* [4] *Laboratoire de Chimie de la Matière Condensée, Faculté de Polydisciplinaire, Université Sidi Mohamed Ben Abdellah, Taza- Maroc.*
* *contact_ parpot@quimica.uminho.pt*

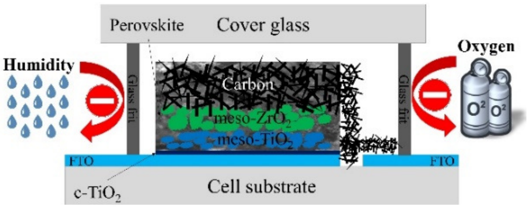


Textile dyes are one of the most important contaminants of the superficial water resources. Their removal from water bodies constitutes a priority to guaranty water quality. Electrodegradation of Congo Red dye was carried out using modified electrodes prepared by the deposition of iron(III)-zeolite on Carbon Toray. The sample iron(III)-zeolite was prepared by ion-exchange method with a solution of iron(III) using NaY$_{nano}$ as parent zeolite, with small particles, 150 nm. Fe(III)NaY$_{nano}$ was characterized by SEM/EDX and XRD techniques. The introduction of iron by ion exchange method do not modified the morphology of the zeolite but affect the zeolite structure, as prove by the structural characterization results from XRD. However, cyclic voltammetry studies show that iron-zeolite modified electrode is stable in the experimental conditions. The complete degradation of Congo Red dye was achieved by electrochemical route without the use of acid and hydrogen peroxide in reactional medium.

[P-EE13]

Hermetic encapsulation of hole transport-free perovskite solar cell

*S. Emami, D. Ivanou, A. Mendes**
LEPABE- Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculdade de Engenharia, Universidade do Porto, rua Dr. Roberto Frias, 4200-465 Porto, Portugal.
** mendes@fe.up.pt*

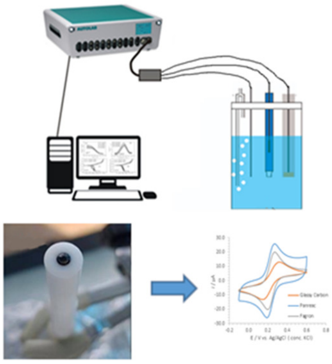


Perovskite solar cells (PSCs) are the most recent emerging photovoltaic (PV) devices. The power conversion efficiency (PCE) of PSCs has rapidly increased from 3.8 % to 23.3 % within the last 10 years. To date, most of the research efforts were focused on improving the PCE of PSCs while the long-term stability of this class of PV remained an enormous challenge. Conventional PSCs include an electron transport layer (ETL), perovskite light absorber and hole transport material (HTM). Since the perovskite layer transports electrons and holes by itself, PSCs can be also fabricated without HTM. Lower production cost and scalable fabrication of HTM-free PSCs make them favorable for commercialization. Perovskite degrades when exposed to humidity and oxygen. Here, a low temperature hermetic encapsulation for HTM-free PSCs that retained 96 % of its initial performance after 23 days is reported. Moreover, the encapsulated cell showed no loss in performance in water immersing test.

[P-EE14]

Electrochemical characterization of commercial activated carbons

N. Nunes[1,2]*, *R. Elvas-Leitão*[1,2], *A. Martins*[1,2]
[1] *Centro de Química e Bioquímica, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade de Lisboa, Ed. C8, Campo Grande 1749-016 Lisboa, Portugal;* [2] *Área Departamental de Engenharia Química, Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, R. Conselheiro Emídio Navarro, 1, 1959-007 Lisboa, Portugal.*
** nnunes@deq.isel.ipl.pt*

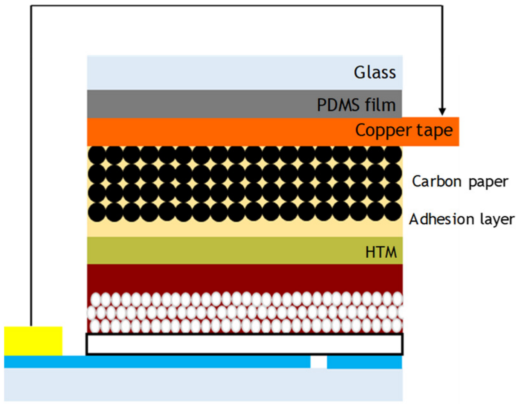


This work deals with the electrochemical characterization of two commercial activated carbons, with distinct textural properties, through cyclic voltammetry, using modified electrodes made by the deposition of activated carbons' samples on a glassy carbon electrode surface. The obtained electroactive surface areas are confronted with previously determined gas and liquid phase adsorption parameters as well as with their surface chemistry by point of zero charge (pH_{pzc}) determination. The results obtained show that despite having very distinct textural parameters, the electroactive surface areas of the two carbon samples are quite similar suggesting that the electrocatalytic properties of carbon-based materials depend on the interaction of electroactive species with the surface's chemical groups of this type of materials.

[P-EE15]

Preparation of carbon-based electrodes to be used as back-contact in perovskite solar cells

*A. C. Teixeira, L. Andrade**, A. Mendes*
LEPABE - University of Porto, Rua Dr. Roberto Frias s/n, Porto, Portugal;
** landrade@fe.up.pt*

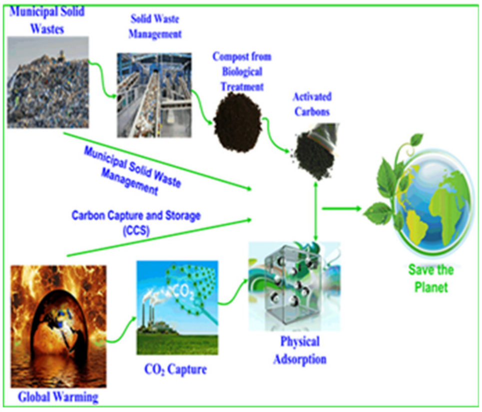


Perovskite solar cells (PSC) are an emerging photovoltaic technology with a great potential to revolutionize the photovoltaic field with a very rapid growth from 3.8% power conversion efficiency to 23.3% in just 10 years. PSCs present low-cost, easy fabrication processes and display special features for building-integrated photovoltaics. However, there are still limitations hindering its commercialization such as the complete cell encapsulation and the expensive back-contact made of gold. Carbon papers are currently used in proton-exchanged membrane fuel cells; this study presents a pioneer work using carbon papers as back-contact in solar cells. In this approach, different adhesion layers were tested to enhance the interfacial contact between the carbon paper and the hole transport material of the PSC and two different carbon papers were studied to perceive the influence of the paper characteristics. A maximum power conversion efficiency of ~7% was reached with the best configuration.

[P-EE16]

Thermally and chemically activated biochar obtained in mechanical biological treatment plants for carbon dioxide adsorption

M. Karimi[1,2,3,], P. Brântuas[1,3], A. Henrique[1, 3], C. Gonçalves [2], J.A.C. Silva [2,3], A.E. Rodrigues [1]*
[1] Porto University, Rua Dr. Roberto Frias, S/N, 4099-002, Porto, Portugal; [2] Polytechnic Institute of Braganca, Campus de Santa Apolonia, 5300-857 Braganca, Portugal; [3] Centro de Investigação de Montanha (CIMO), 5300-253 Bragança, Portugal;
** pedrobrantuas@ipb.pt*

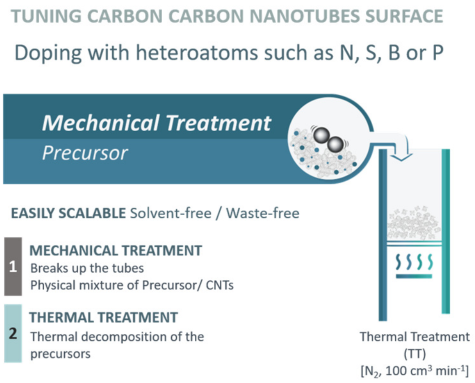


In this study, based on the scopes of CCS strategy and municipal solid waste management, a novel Integrated Environment Management (IEM) strategy has been proposed. In this way, the obtained compost in the mechanical biological treatment from municipal solid wastes has been considered as a source of adsorbents for CO_2 capture. In this way, the maturated compost waste was modified by liquid phase treatment with sulfuric acid and thermal treatment at 800 ^{0}C. Then, the prevalent operational conditions of post-combustion processes have been considered to find the best prepared samples for CO_2 capture.

[P-EE17]

Metal-free carbon nanotubes as catalysts for wet air oxidation of oxalic acid: The role of S, B and P heteroatoms

R.P. Rocha, O.S.G.P. Soares, J.J.M. Órfão, M.F.R. Pereira, J.L. Figueiredo*
Laboratory of Separation and Reaction Engineering—Laboratory of Catalysis and Materials (LSRE-LCM), Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias s/n 4200-465, Porto, Portugal.
** rprocha@fe.up.pt*

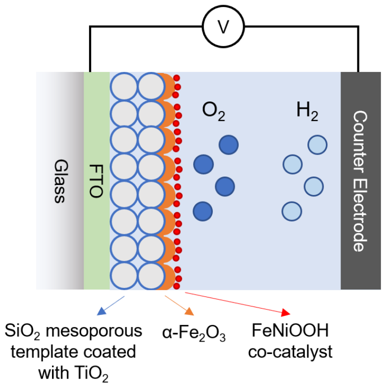


The surface chemistry of carbon nanotubes (CNTs) was modified using a solvent-free methodology involving mechanical and thermal treatments in the presence of precursors of different heteroatoms (S, B, P), promoting significant changes in the CNT textural and chemical properties. The effect of the different heteroatoms on the catalytic performance of the materials was evaluated in the oxidation of oxalic acid by Catalytic Wet Air Oxidation (CWAO), as an alternative to the noble metal and rare earth oxide catalysts traditionally used in this process. Improved catalytic activities were obtained using the P-, B-doped CNTs in oxalic acid oxidation, while S-doped CNTs underperform comparing to the pristine material.

[P-EE18]

Synthesis of high surface area host-guest hematite photoelectrodes for photoelectrochemical cells

F. Francisco[1], P. Dias[1], J. Azevedo[1,2,], A. Mendes[1]*
[1]LEPABE - Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal; [2]IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia, Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal;
**jcazevedo@fe.up.pt*

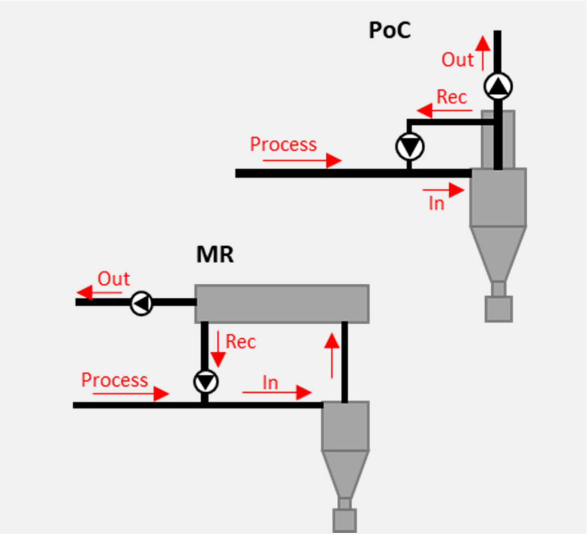


Hematite is a promising semiconductor material for photoelectrochemical devices, due to its abundance, low cost, excellent stability and suitable bandgap (*ca.* 2.1 eV). However, the low mobility of minority carriers (holes) and the fast electron-hole recombination kinetics compared to the light extinguish coefficient, are challenges to overcome; nanostructuring and coating the surface of hematite were the strategies used in the present study for enhancing the performance of this photoelectrode. A thin mesoporous SiO_2 host template (*ca.* 193 nm) was synthesized and optimized, using particles with a surface area of *ca.* 141.6 $m^2 \cdot g^{-1}$, and coated with an intermediate conductive layer of TiO_2 by atomic layer deposition. Finally, a hematite guest thin film was deposited by spray pyrolysis on the prepared host structure, and after coating a FeNiOOH co-catalyst a photocurrent-density of *ca.* 0.98 $mA \cdot cm^{-2}$ at 1.45 V_{RHE} was obtained, showing a lower onset potential of *ca.* 0.70 V_{RHE}.

[P-EE19]

Increasing cyclone performance with an optimized Post-Cyclone recirculator: ReCyclone® MHV

J. Rocha[1], *J. Paiva*[1,2*], *R. Salcedo*[1,2]
[1] *Advanced Cyclone Systems, SA, R. Vilar, 235, Ed. SCALA, 3Esq, 4050-626, Porto, Portugal;* [2] *Faculdade de Engenharia,, R. Dr. Roberto Frias, s/n, 4200-465 Porto Portugal*
**julio.paiva@acsystems.pt*

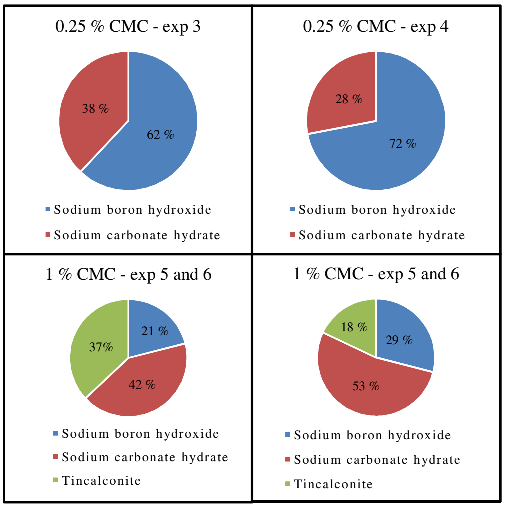


Cyclones are gas/solid separator devices, highly used for the recovery of raw materials and to comply with particle emission limits. Previous works show that tangential inlet, reverse-flow cyclones can be coupled with straight-through concentrators (MR) to increase overall efficiency. The complete setup is named ReCyclone®. On the other hand, pressure drop also increases, negatively affecting the energy efficiency of the system.Unlike mechanical recirculation, post-cyclone systems take advantage of the remaining swirl on the cyclone vortex finder. Post-cyclone systems are mechanical devices designed to increase overall efficiency and energy recovery, by partially recirculating the outlet vortex flow. The results showed an improvement of the cyclone performance when coupled with post-cyclone devices as compared to the MR or to the single cyclone setups. The use of recirculation shows better efficiencies than the single cyclone, at equivalent cyclone inlet velocities.

[P-EE20]

Catalytic hydrolysis of $NaBH_4$ for hydrogen synthesis: study of the by-product of reaction

D. L. Silva[1], *H. X. Nunes*[1], *C. M. Rangel*[2], *A. M. F. R. Pinto*[1,*]
[1]*CEFT – Transport Phenomena Research Center, Chemical Engineering Dpt., Faculty of Engineering University of Porto, Porto, Portugal;* [2]*Solar Energy Unit, LNEG – Nacional Laboratory of Energy and Geology, Lisboa, Portugal.*
** apinto@fe.up.pt*

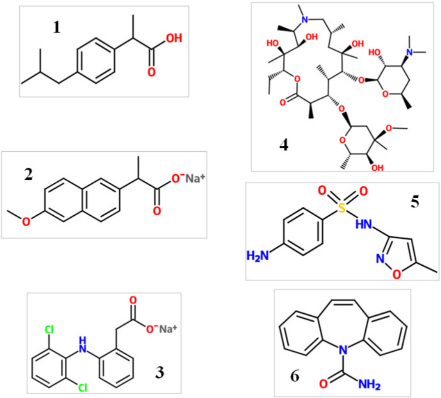


The negative effects of excessive use of fossil fuels are visible today more than ever and the search for alternative and clean energy sources is essential for the future of the planet. Hydrogen can be that alternative. One way to produce and store hydrogen is to use sodium borohydride ($NaBH_4$). It has a high hydrogen content (10.8 wt. %) and, when hydrolyzed, releases it at a moderate pressure and temperature. However, a by-product, sodium metaborate**,** is formed. Due to the excessive cost of $NaBH_4$, its regeneration is essential to be used as a viable method for hydrogen production and storage. In this study, the influence of additive sodium carboxymethyl cellulose was reported. It was observed the formation of $NaB(OH)_4$, $Na_2CO_3 \bullet H_2O$ and $Na_2B_4O_5(OH)_4 \bullet (H_2O)_{2.67}$. $NaB(OH)_4$ is a rearrangement of the sodium metaborate molecules and $Na_2B_4O_5(OH)_4 \bullet (H_2O)_{2.67}$ is tincalconite, a less hydrated form of borax. These are promising results for the regeneration of $NaBH_4$.

[P-EE21]

Monitoring of emerging micropollutants in hydric media in Bragança district

A. Nemoto[1,2], *M. Gonçalves*[2], *A. Ribeiro*[1], *P. Brito*[1], *A. Queiroz* [1,*]
[1]*Mountain Research Center (CIMO), Polytechnic Institute of Bragança, Campus de Sta. Apolónia, 5300-253 Bragança, Portugal;*
[2] *Technological Federal University of Paraná, R. Rosalina Maria Ferreira - 87301-899, Campo Mourão, Brazil;*
**amqueiroz@ipb.pt*



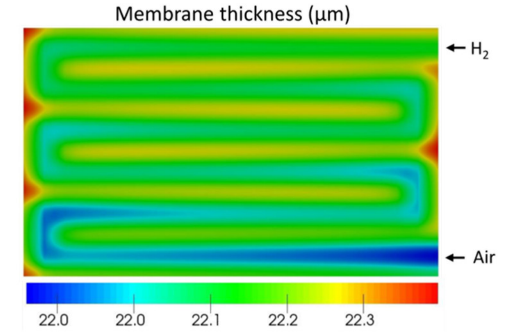
1 Ibuprofen, 2 Diclofenac Sodium, 3 Naproxen Sodium, 4 Azithromycin, 5 Sulfamethoxazole, 6 Carbamazepine

This work aims to develop and validate a method for the quantification and monitoring of emerging micropollutants belonging to the class of pharmaceuticals and personal care products (PPCP´s) in several hydric media from Bragança district, Portugal. Six pharmaceutical drugs were selected for this study, namely, ibuprofen, diclofenac, naproxen, azithromycin, sulfamethoxazole and carbamazepine and belongs to three different subclasses that were worldwide prescribed: three anti-inflammatory, two antibiotics and one antiepileptic, respectively. These compounds were chosen after searching which compounds could be more frequently medical prescribed in Bragança, based on related studies associated with regions with similar socioeconomic data. The next step will be the selection of an extraction and an instrumental method of analysis, as well as the selection of the samples collection points in Bragança and to perform some preliminary monitoring of the referred emerging micropollutants.

[P-EE22]

Numerical simulation of the membrane chemical degradation in a PEM fuel cell

R.B. Ferreira[1,*], *D.S. Falcão*[1], *A.M.F.R. Pinto*[1]
[1] *Transport Phenomena Research Center (CEFT), Chemical Engineering Department (DEQ), Faculty of Engineering of University of Porto (FEUP), Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;*
** rferreira@fe.up.pt.*



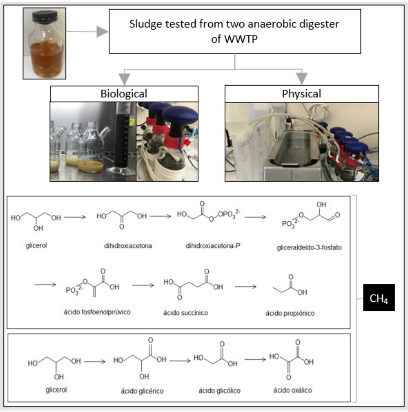
Membrane thickness along the active area of a 2.4 cm^2 cell, after 4000 hours of stationary operation at 0.70 V. The initial thickness of the membrane before degradation is 25.4 μm.

The durability of proton exchange membrane (PEM) fuel cells is a key aspect that still hampers the generalized commercialization of these devices. In particular, the chemical degradation of the membrane is one of the most common failure modes of a stack. In this work, a numerical model is presented that predicts the membrane degradation and its effect on the cell electrical output, as well as the locations along the active area where the membrane degrades most. Semi-empirical laws developed and validated based on experimental results are used to create a membrane degradation sub-model that is incorporated into a commercial PEM fuel cell model. Simulations were conducted at various operating conditions and their effects on the membrane degradation and cell performance are discussed. It is also shown the spatial variation of the membrane thickness after degradation (see Graphical Abstract on the left) and its relation with the local operating conditions.

[P-EE23]

Treatment and energy valorization of residual glycerol in a perfectly mixed batch reactor

L.O. Paulista[1], *R. Boaventura*[1], *V.J.P. Vilar*[1], *A.L.N. Pinheiro*[2], *R.J.E. Martins*[1,3,*]
[1] LSRE-LCM, Faculty of Engineering of the University of Porto, Rua Dr. Roberto Frias, s/n 4200-465, Porto, Portugal; [2] Federal Technological University of Paraná, Estr. dos Pioneiros, 313, Jardim Morumbi, 86036-370, Londrina - PR, Brasil; [3] School of Technology and Management - Polytechnic Institute of Bragança, Campus de Santa Apolónia, 5300-253, Bragança, Portugal.
** rmartins@ipb.pt*

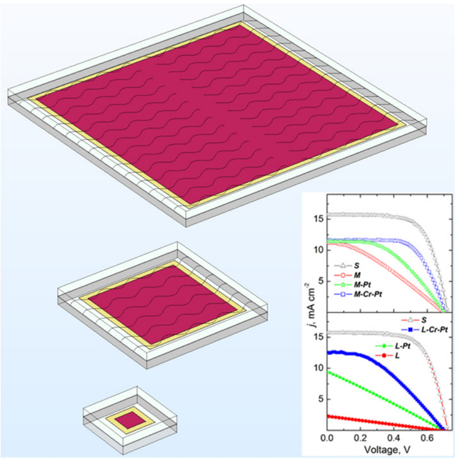


The anaerobic digestion of the crude glycerol from the production of biodiesel is an alternative for methane production. The high organic load of crude glycerol can cause an inhibition of microorganisms. Ultrasound promotes the breakdown of the cell wall and membrane, releasing intracellular material that favors biodigestion. In addition, such microorganisms can produce lipases capable of degrading other impurities contained in the residual glycerol, such as long chain fatty acids. The aim of this study is to improve the anaerobic digestion of glycerol through physical (ultrasound) and biological (*Aspergillus niger* and *Escherichia coli*) pretreatments. The results indicate that the use of ultrasound improved methane generation by 23% for a lower concentration of glycerol (2%). There were also improvements from the use of *A. niger* in 1.7% glycerol. For the concentration of 3.2% glycerol and the use of *E.coli* in all experiments caused inhibition of the methanogenic microorganisms.

[P-EE24]

Boosting the efficiency of large area dye sensitized solar cells

D. Ivanou, J. Capitão, J. Maçaira, A. I. Pereira, A. Mendes
LEPABE, Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto
**jeffreycap@fe.up.pt*

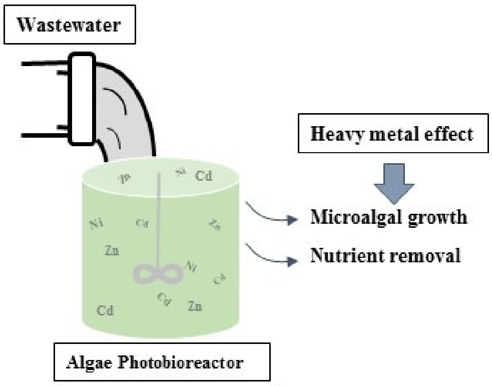


Transparent conducting glass substrates with embedded chromium conducting lines were produced for improving current collection in large area photoanodes of DSSCs. Polarization measurements revealed passivity of Cr in back electron recombination with iodine electrolyte. Collectors were electrochemically deposited beneath glass surface creating grooves in the FTO-glass by photolithography assisted wet etching. Robust adhesion of Cr lines to glass up to 500 °C was achieved. DSSCs photoanodes of 2.5×2.5 cm^2 and 6.5×6.5 cm^2 were assembled using Cr-embedded FTO-glasses resulting in power conversion efficiencies of 5.3 % and 3.6 % respectively; it outperforms the cells with blank FTO glass substrates, mainly due to the improvement of the filling factors. EIS revealed significant decrease of series and electron transfer resistances in the photoanodes assembled on Cr-embedded FTO glass. When aged naturally, the cells with Cr current collectors maintained their efficiency for more than 3000 h.

[P-EE25]

Inhibition effect of heavy metals in microalgal growth and nutrient uptake in wastewaters: an experimental and mathematical approach

F.M. Santos[1,2]*, L.P. Mazur*[2,3]*, D.A. Mayer*[3]*, V.J.P. Vilar*[2]*, J.C.M. Pires*[1]*
[1]*Laboratory for Process Engineering, Environment, Biotechnology and Energy (LEPABE), Chemical Engineering Department, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465, Porto, Portugal;* [2]*Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Chemical Engineering Department, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465, Porto, Portugal;* [3]*Laboratory of Mass Transfer, Department of Chemical Engineering and Food Engineering, Federal University of Santa Catarina (UFSC), PO Box 476, CEP 88040-900 Florianópolis, SC, Brazil.*
**jcpires@fe.up.pt*

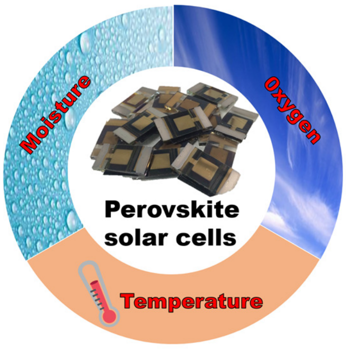


Microalgae bioremediation appears as a low cost treatment of wastewaters. Depending on effluent source, inhibitory compounds (e.g. heavy metals) may reduce microalgal growth and nutrients (N and P) removal. Therefore, this paper aims to evaluate the heavy metal (Cd, Ni and Zn) effect in the cultivation of *Chlorella vulgaris* in simulated wastewater. A maximum growth rate of 0.34 d^{-1} was observed in Cd and Zn presence. With Cd, the maximum biomass productivity (98.1 mg·L^{-1}·d^{-1}) and higher removal efficiencies of nitrogen (90.6%) and phosphorus (98.7%) were achieved. Ni causes the highest inhibition percentages (>88%). Regarding metals removal, the best efficiency was obtained in Zn culture (85.4%). Kinetic and the equilibrium were described by a Monod model and Langmuir isotherm, respectively. This work presents relevant results for the integration of microalgae culture in the wastewater treatment containing heavy metals, improving this process in different sectors of economic activity.

[P-EE26]

Impact of environmental conditions in perovskite solar cells: temperature, oxygen and moisture

*I. Mesquita, L. Andrade***, A. Mendes*
LEPABE - Faculdade de Engenharia, Universidade do Porto, rua Dr. Roberto Frias, 4200-465 Porto, Portugal.
** landrade@fe.up.pt*

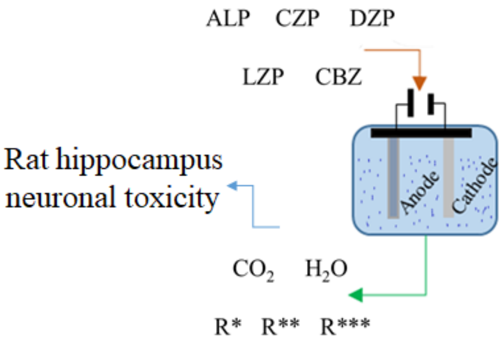


Perovskite solar cells technology have emerged, in the last few years, as an attractive candidate for photovoltaic applications due to their exceptional optoelectronic properties. However, the devices still suffering of a lack in stability at high temperatures and in contact with oxygen and moisture, what is delaying their commercialization. This work aims at to help understanding the impact of different environmental elements in the preparation and operation of the perovskite solar cells, reporting not only the impact of oxygen and humidity during the fabrication of devices, but also the impact of temperature during their operation. The results led us to conclude that while the temperature affects mostly the hole extraction layer due to additives evaporation, the humidity and oxygen affect mainly the morphology of the perovskite layer and its stability during time.

[P-EE27]

Degradation of benzodiazepines and carbamazepine by electrochemical oxidation using boron doped diamond electrode and effects on neuronal toxicity

M. Bosio[1,4,*], *B. Souza*[1,4], *E. Saggioro*[2], *M. Dezotti*[1], *J. Bassin*[1], *E. Quinta-Ferreira*[3], *R. Quinta-Ferreira*[4]
[1] Programa de Engenharia Química - PEQ/COPPE, Universidade Federal do Rio de Janeiro, P.O. Box 68502, 21941-972, Rio de Janeiro, RJ, Brazil [2] *Sanitation and Environment Health Department, Sergio Arouca National School of Public Health, Oswaldo Cruz Foundation, Avenida Leopoldo Bulhões, 1480, Rio de Janeiro – 21041-210, Brazil;* [3] *Center for Neurosciences and Cell Biology and Physics Department, University of Coimbra, Rua Larga, Coimbra – 3004-516, Portugal; CIEPQPF – Chemical Engineering Processes and Forest Products Research Center, Department of Chemical Engineering, University of Coimbra, Rua Sílvio Lima, Coimbra – 3030-790, Portugal;*
** morganabosio@yahoo.com.br*



Currently, wastewater discharge has become a serious concern due to the potential risk for the ecosystem. Continued exposure to contaminated water, even at low concentrations, can cause negative effects on human health and environment. Some pharmaceutical substances are not fully eliminated under conventional wastewater treatment. Therefore, new technologies are required to remove these compounds, such as advanced oxidative processes. Here, the electrooxidation process was used to degrade five pharmaceutical compounds: alprazolam (ALP), clonazepam (CZP), diazepam (DZP), lorazepam (LZP) and carbamazepine (CBZ). The oxidation ability of the system was evaluated varying the pH, current density and aqueous matrix. The best results were obtained with 0.3 A, 1.5 g.L^{-1}NaCL, pH 7 and ultrapure water, leading to complete degradation of ALP, CZP, DZP, LZP, and CBZ. Toxicity tests showed a decrease in ROS (Reactive Oxygen Species) production.

[P-EE28]

Drying sewage sludge with coal fly ash for producing a soil amendment

L. A. Gomes[1,2*], *R. Lopes*[1], *J.C. Góis*[3], *M.J. Quina*[1]
[1]*CIEPQPF, Chemical Process Engineering and Forest Products Research Centre. Department of Chemical Engineering, University of Coimbra, Portugal;* [2]*IFB - Federal Institute of Education, Science and Technology of Brasília - IFB, Campus Ceilândia, Brasília - Federal District, Brazi*l; [3]*Association for the Development of Industrial Aerodynamics, Department of Mechanical Engineering, University of Coimbra, Coimbra, Portugal.*
**luciano.gomes@ifb.edu.br*

The high quantities of sewage sludge (SS) and coal fly ash (CFA) produced require an adequate management for protecting human health and the environment. This study aims to investigate the possibility of using CFA as SS drying adjuvant for producing a soil amendment.The study involved the characterization of SS and CFA at a physical and chemical level. The drying process of small cylinders, for several combinations of SS:CFA (100:0 - control; 95:5; 90:10 and 85:15) at different temperatures (40, 70, 100 and 130 ºC) was investigated. The dynamic model of the drying process was based on the Fick law and an infinite length was assumed for the small cylinders. The kinetics analysis showed that as the quantity of CFA increases the rate of drying is faster. The effective diffusion coefficient and other relevant parameters were determined for each thermal drying condition. The results showed that the drying process of SS with small quantities of CFA may be a route for valorizing these wastes in agricultural soil.

[P-EE29]

Biodiesel production using nanocatalyst from calcium waste materials

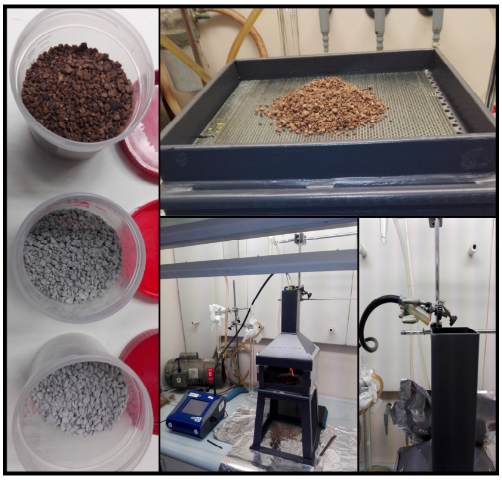
S. Santos[1,*]*,L.C.S.Nobre*[2]*, J. Puna*[1,3]*, J. Gomes*[1,3]*, R. Quinta-Ferreira*[4]*, J. Bordado*[1]
[1] *CERENA, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1, Lisboa, 1049-001, Portugal;* [2] *CQE, Universidade de Lisboa, Lisboa, Portugal;* [3] *Instituto Superior de Engenharia de Lisboa, R. Conselheiro Emídio Navarro, 1, Lisboa, 1959-007, Portugal;*[4] *Faculdade de Ciências e Tecnologias, Universidade de Coimbra, R. Sílvio Lino s/n, Coimbra, 3030-790, Portugal.*
** samuelpsantos@tecnico.ulisboa.pt.*

Considering heterogeneous catalysts for transesterification reaction, calcium oxide (CaO) is a widely-used catalyst due to being cheap, non-corrosive, economically benign, easy to handle and having a high basicity compared to homogeneous base catalysts. Using CaO nanocatalysts, it is possible to overcome some of these drawbacks, as they present higher surface area and catalytic activity, thus allowing to achieve a significant improvement on transesterification efficiency. In the present work, CaO from natural sources was micronized using the SAS (Supercritical Anti-Solvent) technique with Supercritical CO_2. The obtained nanocatalysts were then analysed by SEM and DLS. The transesterification of soybean oil into biodiesel using these catalysts was tested at 60º C with methanol reflux. Reaction conditions such as reaction time, methanol/oil molar ratio and catalyst loading amount were studied as well as its effect on the yield of the triglyceride conversion into FAME.

[P-EE30]

Preliminary tests on the use of additives to decrease fine particles emission in biomass combustion

J.A.D. Condeço[*1]*, S. Hariharakrishnan*[1]*, N. Canha*[2]*, S.B. Pereira*[3]*, M. Costa*[3]*, J. Bordado*[1]*, J.M.N. Correia*[1]
[1] *CERENA, Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal;* [2] *C²TN, Centro de Ciências e Tecnologias Nucleares, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal;* [3] *IDMEC, Departamento de Engenharia Mecânica, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal;*
** jose.condeco @tecnico.ulisboa.pt.*

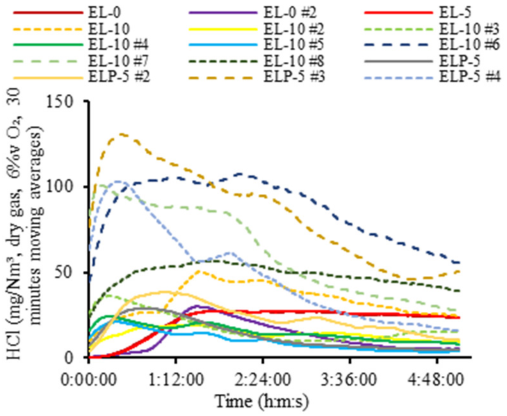


This work describes the results of the effect of additives on PM (Particulate Matter) emission in pinewood biomass combustion. Thus, preliminary combustion tests of pinewood biomass with and without additives were carried out to evaluate the effectiveness of these additives on the reduction of fine particles emission. The additives tested were CaO, TiO_2 and Montmorillonite $(Na_{0.2}Ca_{0.1}Al_2Si_4O_{10}(OH)_2(H_2O)_{10})$. The additives concentrations studied were 1.5%, 3% and 4.5% (w:w) and an apparatus was designed to perform these preliminary tests. PM concentration was measured using a DustTrak DRX Aerosol Monitor 8533 (TSI, Inc., Shoreview, Minn.) that allows the continuous measurement of PM_1, $PM_{2.5}$, PM_4 and PM_{10} µm particles (particles with an aerodynamic diameter of 1, 2.5, 4 and 10µm). The obtained results indicate that these additives contributed to the reduction of PM1 concentration in the flue gas and that a concentration of 3% (w:w) seems to be a good choice to be deeply studied in the drop tube furnace to be carried out in a near future.

[P-EE31]

Co-combustion of residual forest biomass derived from *Eucalyptus* with sludge from wastewater treatment in the pulp and paper industry: NO and chlorine emissions

D.T. Pio[1,], L.A.C. Tarelho[1], T.F.V. Nunes[1], M.A.A. Matos[1]*
[1] Department of Environment and Planning & Centre for Environmental and Marine Studies (CESAM), University of Aveiro, Campus Universitário de Santiago 3810-193, Aveiro, Portugal;
** danieltp@ua.pt, ltarelho@ua.pt.*

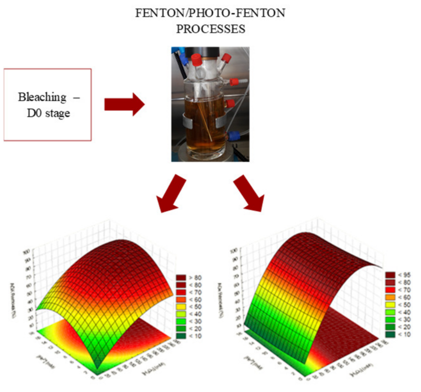


Residual forest biomass mixed with different mass percentages of primary and secondary sludge from the pulp and paper industry was studied as fuel for combustion in a pilot-scale bubbling fluidized bed. The main objective was the determination of sludge addition influence on the overall process and on the composition of the exhaust gases, with emphasis on chlorine emissions, namely present in the solid phase (fly ashes) and in the gaseous phase (HCl), and NOx emissions. The co-combustion process of residual forest biomass with primary sludge (up to 5%wt) and secondary sludge (up to 10%wt) was successfully demonstrated as a valid energy valorization option for the sludges. Except specific cases, no significant emissions increase of NOx, CO or HCl were found with the addition of sludge. In fact, HCl emissions decreased due to an increase in the chlorine retention in ashes caused by the high inorganic content present in the sludges.

[P-EE32]

Optimization of Fenton/photo-Fenton processes for AOX removal from real pulp and paper bleaching wastewater

J.P. Ribeiro[1], C.C. Marques[1], I. Portugal[2], M.I. Nunes[1,]*
[1] CESAM - Centre for Environmental and Marine Studies/Department of Environment and Planning, University of Aveiro, Campus Universitário de Santiago 3810-193, Aveiro, Portugal; [2] CICECO - Aveiro Institute of Materials/Department of Chemistry, University of Aveiro, Campus Universitário de Santiago 3810-193, Aveiro, Portugal;
** isanunes@ua.pt*



AOX Removal by Fenton (left) and photo-Fenton (right) from PP bleaching wastewater

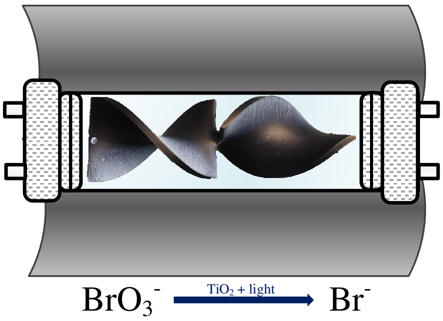
D_0 bleaching wastewater stream from a real pulp and paper industry with 124 mg.L^{-1} AOX content was treated by Fenton and photo-Fenton processes. The aim was to optimise the operational conditions [H_2O_2], [Fe^{2+}] and treatment time for AOX removal, within the following ranges: 25-250 mM H_2O_2, 1-16 mM Fe^{2+} and 5-30 min of treatment time. Effect on COD and colour was also checked, considering initial concentrations of 4.16 g O_2 .L^{-1} and 1.27 g.L^{-1} Pt, respectively. Central composite experimental design was used to plan the experiments. Both Fenton and foto-Fenton processes showed potential to remove AOX from D_0 bleaching wastewater, achieving additional removal of COD and colour. For 10 minutes of treatment, photo-Fenton achieved higher AOX removal than Fenton process: 95% against 85%. At those optimal conditions, and for the same treatment time, the COD and colour removals attained were also higher for photo-Fenton.

[P-EE33]

Photocatalytic reduction of bromate in fresh waters using a static mixer as photocatalyst support

*D. Morais**, *F.Moreira, R. Boaventura, V. Vilar*

Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.
** daniela.morais@fe.up.pt.*

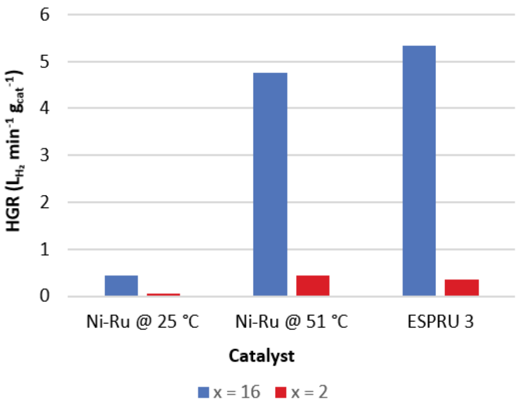


The current study focuses on the photocatalytic reduction of bromate (BrO_3^-) in fresh waters using a tubular photoreactor containing a Kenics® static mixer (SM) coated with a TiO_2-P25 thin film. Two fresh water samples from a drinking water treatment plant (DWTP) were used: one collected downstream ozonation process (DWO) and the other collected downstream ozonation followed by flocculation and flotation/filtration (DWF). BrO_3^- reduction rates were assessed for both samples and further compared with a synthetic water prepared with ultrapure water (UPW) at different pH values. Furthermore, the effect of humic acids (HAs) on BrO_3^- reduction was evaluated. Overall, reaction rates using DWF were higher than the ones obtained for DWO and UPW only. Carbonate species present in higher contents enhance BrO_3^- reduction. Addition of organic matter in the form of HAs proved to improve the photocatalytic reduction of BrO_3^-. The highest BrO_3^- reduction rate was attained for UPW spiked with HAs.

[P-EE34]

The effect of Ni-Ru supported catalyst in the sodium borohydride catalytic hydrolysis for hydrogen generation.

H. X. Nunes[1], *C. M. Rangel*[2], *A. M. F. R. Pinto*[1,*]
[1]*CEFT – Transport Phenomena Research Center, Chemical Engineering Dpt., Faculty of Engineering University of Porto, Porto, Portugal;* [2]*Solar Energy Unit, LNEG – Nacional Laboratory of Energy and Geology, Lisboa, Portugal.*
** apinto@fe.up.pt*

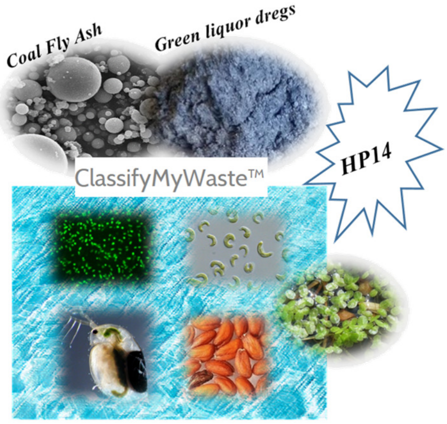


Climate changes and fossil fuel depletion are the main reasons leading to hydrogen technology. Since early 2000's the chemical hydrides, in particular sodium borohydride ($NaBH_4$), hydrolysis reaction attracted much attention as a hydrogen carrier due to its high hydrogen storage capacity (10.8%), safe handling and fast kinetics of H_2 release. Despite the many efforts dedicated to understanding and increase the hydrolysis reaction efficiency through the research and development of a suitable catalyst, there are some issues that need to be addressed. The performance of Ni-Ru supported catalysts in the $NaBH_4$ hydrolysis was studied both in stabilized hydrolysis (x = 16) and alkali-free hydrolysis (x = 2) reactions. The results present high hydrogen generation rates, at uncontrolled room temperature, that compete directly with the rates previously obtained with a Ni-Ru unsupported catalyst, which are advantages to portable applications.

[P-EE35]

Assignment of hazardous characteristics to wastes: HP14 ecotoxicity

B.S. Bandarra[1], *L.A. Gomes*, [1,2], *J.L. Pereira*·[3], *F J.M. Gonçalves*[3], *R.C. Martins*[1], *M.J. Quina*[1, *]
[1] *CIEPQPF, Chemical Process Engineering and Forest Products Research Centre. Department of Chemical Engineering, University of Coimbra, Portugal;* [2] *IFB - Federal Institute of Education, Science and Technology of Brasília - IFB, Campus Ceilândia, Brasília - Federal District, Brazil;* [3] *CESAM, Department of Biology, University of Aveiro, Portugal;*
**guida@eq.uc.pt*

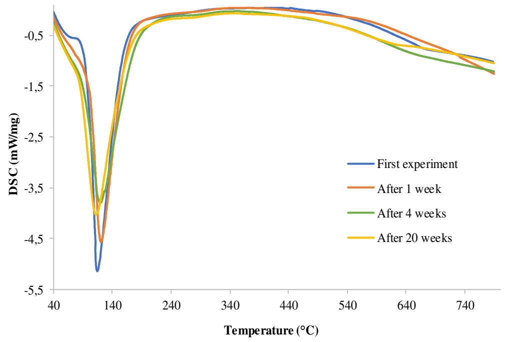


Wastes must be managed correctly to protect human health and the environment. The main objective of this study was to assess the suitability of a methodology to classify wastes in respect to the hazard property HP14: ecotoxicity. Two case studies were addressed: coal fly ash (CFA) and green liquor dregs (GLD). To evaluate HP14, besides a chemical approach using the ClassifyMyWaste™ software, the focus was in a battery of biotests with species of different trophic levels. Thus, five different organisms were tested in the aquatic environment: the bacteria *Aliivibrio fischeri*, the microalgae *Raphidocelis subcapitata*, the macrophyte *Lemna minor*, the microcrustacean *Daphnia magna* and the plant *Lepidium sativum L.* This work showed that GLD have ecotoxic potential since high inhibition compared to the control was observed in most of the parameters evaluated, but the opposite was found to CFA. The chosen methodology seems to be capable of providing relevant results for HP14 assessment.

[P-EE36]

Thermochemical characterization of tars produced in the context of biomass gasification

D. Santos[1], *D. Pio*[1,2], *D. Silva*[2], *F. Lemos*[1], *L. Tarelho*[2,*], *M.A.N.D.A. Lemos*[1,*]
[1] *CERENA, Departamento de Engenharia Química, Instituto Superior Técnico, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal;* [2] *CESAM, Departamento de Ambiente e Ordenamento, Universidade de Aveiro, Portugal.*
** ltarelho@ua.pt ; mandal@teccnico.ulisboa .pt*

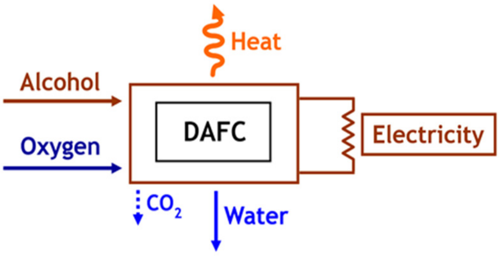


Gasification is a well-developed process for the production of energy and fuels but most of the gasifiers are run on coal as their feedstock. In the context of CO_2 emissions reduction the direct gasification of biomass is gaining increasing interest but there are still several issues that must be solved for this process to gain wider applicability. One of the major problems in biomass gasification is the production of tars that occurs mainly in the pyrolysis stage inside the gasifier. This work is aimed at analyzing the tars that are formed during the pyrolysis stage of biomass feedstock by thermochemical analysis using simultaneous TG/DSC analysis. The results, albeit preliminary, indicate that the TG/DSC analysis can be used to characterize the tars produced, in particular in what concerns the thermochemical reactivity of the heavier components.

[P-EE37]

Performance of a passive and semi-passive direct alcohol fuel cell

C.S. Moreira[1], V.B. Oliveira[1,*], A.M.F.R. Pinto[1,*]
[1]Transport Phenomena Research Center (CEFT), Department of Chemical Engineering, Faculty of Engineering University of Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal.
[*] apinto@fe.up.pt; vaniaso@fe.up.pt

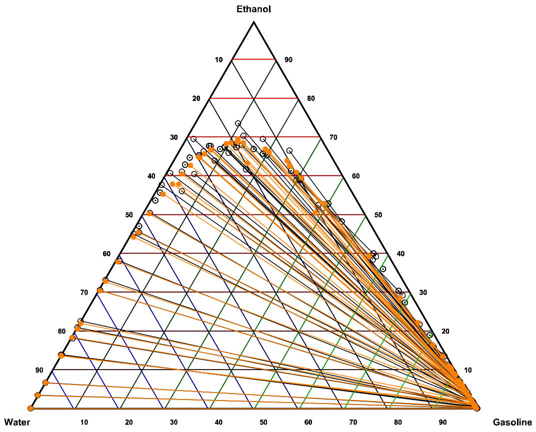


The direct alcohol fuel cells (DAFCs) are a promising technology to replace the conventional batteries in portable applications, since they allow an easy handling, high energy density and are more environmentally friendly. The DAFCs can be categorized in passive, semi-passive and active, according to the reactants feeding system. Passive systems have potential to be implemented in portable electronic devices since they do not require additional power consumption and moving parts. However, active fuel cells offer better performances. Semi-passive DAFCs can combine the best characteristics of both active and passive fuel cells. In this work, the effect of some operational parameters on the performance of a passive and a semi-passive DAFC was evaluated, towards its optimization. The methods used for this purpose were the polarization and electrochemical impedance spectroscopy (EIS) measurements. The polarization measurements allow the identification of the different losses that negatively affect the DAFC performance, while the EIS ones its quantification.

[P-EE38]

Gasohol direct production for energy-efficient bioethanol downstream processing

A.D.S. Nunes[1], J.F.O. Granjo[1,*], B.P.M. Duarte[1,2], N.M.C. Oliveira[1]
[1] CIEPQPF, Department of Chemical Engineering, University of Coimbra, Rua Sílvio Lima, Pólo II, 3030-790 Coimbra, Portugal; [2] Department of Chemical and Biological Engineering, ISEC, Polytechnic Institute of Coimbra, Portugal.
* josegranjo@eq.uc.pt.



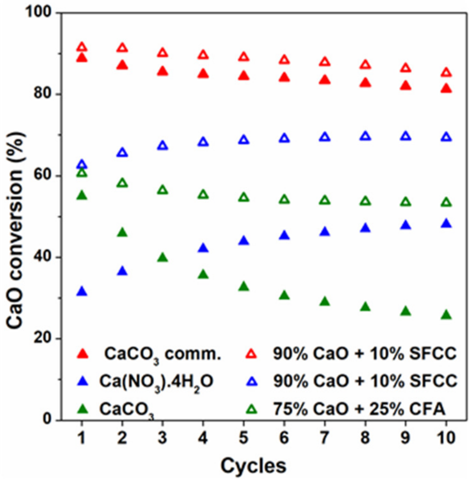
This work addresses the production of gasohol using gasoline as a separation agent, corresponding to an alternative approach to processes that recover and dehydrate ethanol before this is mixed with gasoline. Experimental data was used to build the thermodynamic modeling framework to adequately describe phase equilibrium and predict thermophysical properties. Two configurations for the direct manufacture of E10 gasohol were designed and analyzed. Process 1 is extraction-based whereas Process 2 is extractive distillation-based. Energy requirements were compared against each other and with the most commonly used commercial process where ethanol dehydration is achieved with molecular sieves (Process MS).

The results show that Process 1 is energetically more favorable, consuming on average less 12% than Process MS, for ethanol concentrations in vinasse between 2 and 10 wt%. On average Process 2 also spends less energy than the commercial Process MS, but now only just 2%.

[P-EE39]

Improved sorbents for Calcium looping CO_2 capture in the cement industry: Increasing sintering resistance using waste resources and steam

*P. Teixeira**, *I. Mohamed, C.I.C. Pinheiro, A. Fernandes, M.F. Ribeiro*
QE–Centro de Química Estrutural, Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais 1, 1049-001 Lisboa, Portugal.
** paula.lourenco.teixeira@gmail.com*



Keeping the reactivity and stability of CaO-based sorbents along the cycles of the Ca-looping process is still a challenge. To increase the sorbents sintering resistance, three CaO precursors were dry mixed with wastes. The CaO conversion of original and mixed sorbents was compared. Coal fly ash and spent Fluidized Catalytic Cracking (FCC) wastes were selected due to their silica and alumina composition, as the deactivated sorbents can be used for clinker production. The effect of steam was also studied.

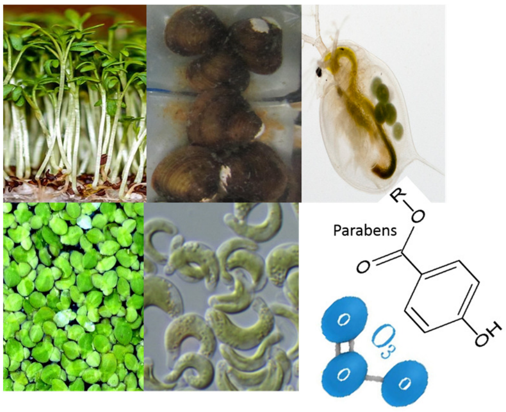
The CaO conversion along the carbonation (700°C) and calcination steps (800ºC for air and 900°C for CO_2 atmosphere) was tested in a thermogravimetric analyzer and in a fixed bed reactor using a gas mixture of 25% of CO_2 balanced in air. The mixed sorbents show higher CaO conversions probably due to the physical barrier created by the added wastes that prevent the sintering.

N_2 sorption and SEM analysis were performed to study the textural and morphologic characteristics of sorbents.

[P-EE40]

On the efficacy of single and catalytic ozonation using volcanic rock in mitigating the ecotoxicity of a parabens mixture

J. Gomes [1,*], *D. Frasson*[1], *J. Pereira*[2], *F. Gonçalves*[2], *L. Castro*[1,3], *R. Quinta-Ferreira*[1], *R. Martins*[1]
[1]*CIEPQPF – Chemical Engineering Processes and Forest Products Research Center, Department of Chemical Engineering, Faculty of Sciences and Technology, University of Coimbra, Rua Sílvio Lima, 3030-790 Coimbra, Portugal.*[2] *Department of Biology & CESAM – Centre for Environmental and Marine Studies, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal.* [3] *Coimbra Polythecnic, ISEC, Rua Pedro Nunes, Quinta da Nora, 3030-199 Coimbra, Portugal.*
** jgomes@eq.uc,pt*



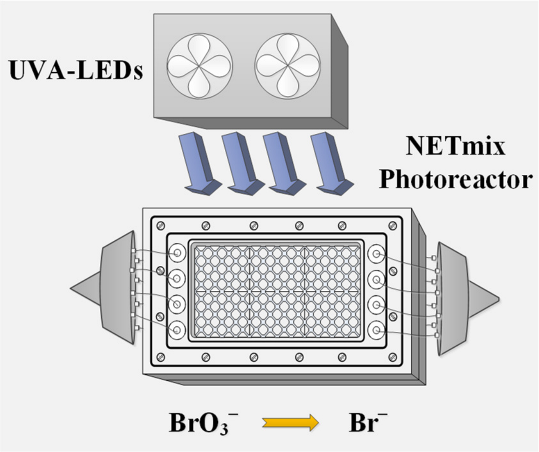
Parabens are widely used as antimicrobial and preservative compounds in pharmaceutical and personal care products. The toxic effect of a mixture of 5 parabens and its degradation products through single and catalytic ozonation was investigated over: cladocerans, microalgae, clams, macrophytes and cress. Parabens were totally removed by both oxidation systems. However, the same was not true regarding toxicity mitigation, since the toxicity of the samples resulting from both treatments was generally higher than that determined for the initial parabens mixture. While catalytic ozonation allows reducing the amount of ozone required for total removal of parabens, the resulting treated solution was more toxic than the sample taken at the endpoint of the single ozonation treatment. The highest amount of ozone used for single ozonation allows the elimination of toxic by-products. Still, the effect of by-products and parabens interaction depends on the species analyzed on the toxicity tests.

[P-EE41]

Bromates removal by heterogeneous photocatalysis in a drinking water treatment plant

*S. Santos**, *L. Paulista, T. Silva, R. Boaventura, M.M. Dias, J.C.B. Lopes, V. Vilar*

Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;
** s.santos@fe.up.pt*

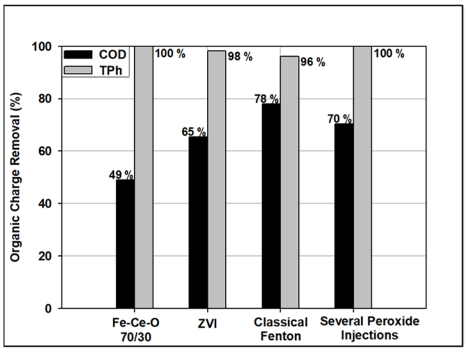


The main goal of this study was to evaluate the removal of bromates from drinking water by heterogeneous TiO_2 photocatalysis using a mili-photoreactor based on the NETmix technology. The channels and chambers of the mili-photoreactor were coated with a TiO_2 thin film by a spray deposition technique. The catalyst surface was illuminated by UVA-LEDs. Water samples from a water treatment plant (WTP), after ozonation (OW) and after ozonation+flocculation+filtration (FW), were used as reaction matrices. Bromate reduction rates were assessed for both water samples at different pH values and then compared with a synthetic water (BrO_3^- solution prepared using UPW). Overall, reaction rates using the OW were higher than FW, except at pH 5.5 where they were similar. Higher [HCO_3^-] and [DOC] for OW samples at pH 6.5 and ~7.5, when compared with FW, showed a positive effect on the reduction rates. Still, bromate reduction rates were higher for the synthetic water than for the waters from the WTP.

[P-EE42]

Comparative studies between homogeneous and heterogeneous Fenton's process – low-cost materials experimentation and alternatives to the classic process

*A.F. Rossi, R.C. Martins, , R.M. Quinta-Ferreira**
Chemical Engineering Department of the Faculty of Sciences and Technology of the University of Coimbra, Rua Sílvio Lima, Coimbra, Portugal.
** rosaqf@eq.uc.pt*



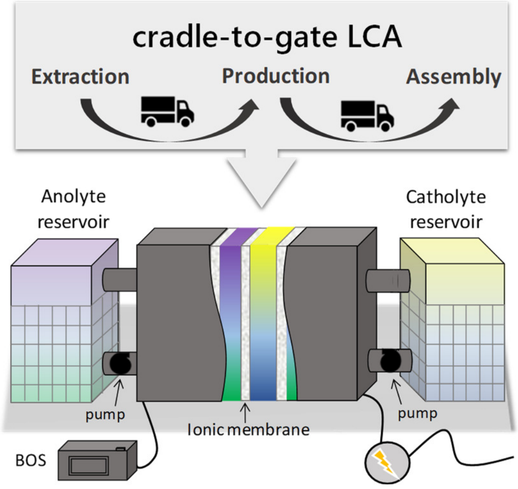
Final comparison regarding organic charge removal results for each kind of procedure.

The efficiency of three ceramic catalysts (Fe-Ce-O, Fe-Cu-O and Fe-Co-O), three low cost materials (zero valent iron, ZVI, from both iron bars and iron cutting shavings and Fenton's sludge) and the homogeneous Fenton's process are put side to side and compared regarding TPh and COD removal from an Olive Mill synthetic wastewater. The best conditions are indicated for each and the most interesting points are highlighted. Being the center of this discussion, the Fenton's oxidative capacities on the remediation of a phenolic synthetic wastewater is exposed. A different approach of the classical Fenton's process is analyzed as an attempt to overcome some of its disadvantages. Several peroxide injections enhanced the procedure's efficiency in organic charge depletion and reduced the major disadvantage of the Fenton's reaction: sludge formation.

[P-EE43]

Life cycle assessment of a vanadium flow battery

J.R. Gouveia[1], A. Monteiro[1], T.M. Mata[1], A Mendes[1], N.S. Caetano[1,2], A.A. Martins[1]*
[1]LEPABE/FEUP, R. Dr. Roberto Frias S/N, 4200-465 Porto, Portugal; [2]ISEP R. Dr. António Bernardino de Almeida 431, 4249-015 Porto, Portugal.
* amartins@fe.up.pt



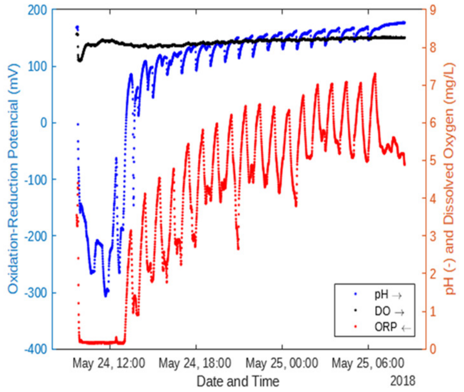
Renewable energy sources are often not fully dispatchable making critical the development of energy storage systems. Among the various options for storing energy easily convertible in electricity, batteries are seen as one of the most promising approaches.

In this work, a life cycle assessment of a prototype 5 kW and 18 kWh vanadium redox flow battery is performed on a cradle-to-gate approach. Primary data from the prototype was used to build the inventory, complemented when needed with information and data from the literature and the EcoInvent V.34 life cycle inventory database. The ILCD 2011 Midpoint+ method was used to estimate the potential environmental impacts. The results show that the environmental hotspots lie mostly in the battery's structural components and materials, in particular the vanadium electrolytes, evidencing the need for alternative or recycled materials preferably produced locally. Moreover, within a cradle-to-gate perspective, there is a need to develop electrolytes with higher energy density and lower usage of sulphuric acid.

[P-EE44]

Nitrogen and COD removal enhancement in a SBR: Influence of using step-feed and indirect parameters monitorization, in a real-time control perspective

I.O. Inocêncio[1], A.G. Nogueira[2], S. Castro-Silva[2,]* R.C. Martins[1], R.M. Quinta-Ferreira[1]
[1] Chemical Engineering Department of the Faculty of Sciences and Technology of the University of Coimbra, Departamento de Engenharia Química, Universidade de Coimbra, Rua Sílvio Lima, 3030-790 Coimbra, Portugal; [2] Adventech – Advanced Environmental Technologies, Lda, Centro Empresarial e Tecnológico, Rua de Fundões 151, 3700-121 São João da Madeira, Portugal.
* sergio.silva@adventech-group.com

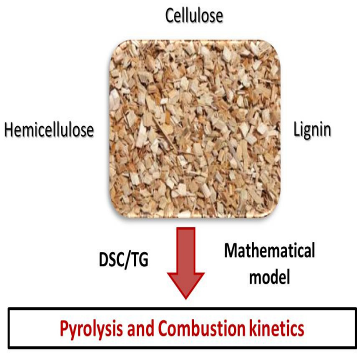


The objective of this work was to investigate a real-time control (RTC) strategy using indirect parameter probes (ORP, pH and DO) in a SBR treating winery effluent. The aim was enhancing N and COD removal and reduce aeration costs in an industrial wastewater treatment plant. The test variables were the duration of each aerobic/anoxic phase and the use of a step-feed approach. Results revealed that increasing the duration of the aerobic and anoxic phases allows a more efficient nitrogen removal, but the use of step-feed decreased both TN and COD removal, obtaining effluents inadequate for discharge. DO breakthrough control point was successfully found both in DO and ORP profiles. Only 3 N control points were found in the study, invalidating the possibility for RTC on N removal, but effluent's nitrogen fulfilled discharge parameters. The results showed strong evidences that RTC based on COD removal is possible by tracking DO breakthrough point, reducing global aeration time in 56 %.

[P-EE45]

Kinetic modelling of the pyrolysis and combustion of woody biomass

*M. Martins[1, *], D. Pokwiczał[1], F. Lemos[1], H. Pereira[2], J. Zuwała[3], T. Iluk[4], M. A. Lemos[1]*
[1] CERENA, Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal; [2] Centro de Estudos Florestais, Instituto Superior de Agronomia, Universidade de Lisboa, Lisboa, Portugal; [3] AGH, Krakow, Poland; [4] Institute for Chemical Processing of Coal, Zabrze, Poland.
**marta.oliveira,martins@tecnico.ulisboa.pt*

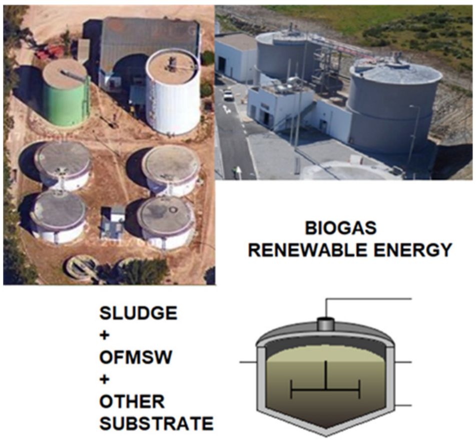


Thermochemical conversion of biomass into energy and feedstock chemical is gaining increasing importance in the current context. Gaining insight on the thermochemical conversion of biomass is very important and constitutes the objective of many research works. In this work, the thermochemical transformation of wooden chips (alder) sample provided by Institute of Coal Chemical Processing in Zabrze (Poland) were studied by, thermoanalytical methods in particular, using Differential Scanning Calorimetry (DSC/TG) technique. Experiments were conducted both under pyrolysis and combustion conditions, at different heating rates (10, 20 and 50 °C/min), in a temperature range from 40 to 800°C. The information was analyzed by means of pseudo-component kinetic models where, as a first approach, the reactions were assumed to be first order.

[P-EE46]

Energy optimization of sludge anaerobic digestion

M. T. Santos[1,], F. Alves[2]*
[1] Área Departamental de Engenharia Química, Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, R. Conselheiro Emídio Navarro 1, 1959-007 Lisboa, Portugal; [2] Área Departamental de Engenharia Civil, Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, R. Conselheiro Emídio Navarro 1, 1959-007 Lisboa, Portugal.
** tsantos@deq.isel.ipl.pt*

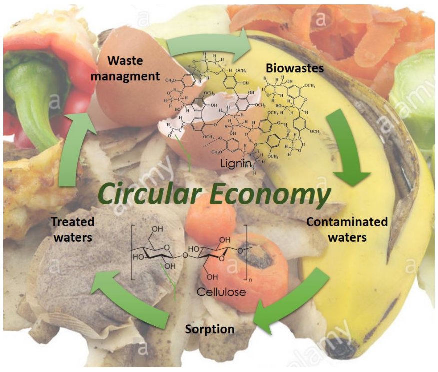


In Portugal the optimization of anaerobic digestion is desirable, however, the sludge amount does not present a great growth potential in volume (or mass), since the country's infrastructure is consolidated. However, there is an opportunity to identify potentials for optimization and valorization of anaerobic digestion stages in the WWTP either by process changes or by incorporation of other substrates. The present work main issue is to analyze the installed capacity and efficiency of the anaerobic digestion process carried out by the WWTP and the possibility of performing an anaerobic co-digestion with other substrates. Also, to determine the potential for energy manufacture by biogas production. Therefore, a survey of existing WWTP was done but due to the high number of WWTP, it was necessary to select some regions, namely center and south of Portugal. As a result it was found that, the energy produced from biogas represents in average from 10 % to 20 % of WWTP of energy needs.

[P-EE47]

Study of Hg^{2+} removal from tap water using different biosorbents

E. Fabre[1,2*], *C. Vale*[3], *E. Pereira*[2], *C.M. Silva*[1]
[1] *CICECO, Department of Chemistry, University of Aveiro, Aveiro, Portugal;* [2] *CESAM, Department of Chemistry, University of Aveiro, Aveiro, Portugal;* [3] *CIIMAR, University of Porto, Porto, Portugal.*
* *elainefabre@ua.pt*

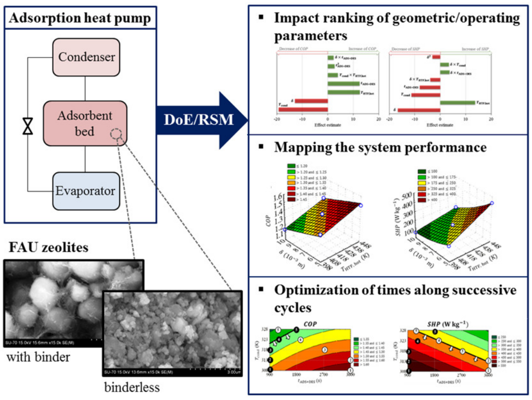


Mercury is one of the most hazardous toxic metals due to its ability of accumulation into the living organism tissues and bioamplification along the food chain. In line with the concept of circular economy, agricultural wastes and industrial by-products have been investigated in order to provide eco-friendly sorbents for water treatment applications. Banana and potato peels, egg shells, *Eucalyptus globulus* bark and coffee wastes were used to remove mercury from tap water solutions. The ability of these biosorbents was evaluated through batch experiments under room temperature and Hg(II) concentration of 50 µg/L. The best performance was achieved by banana peels, which showed removals of mercury(II) in solution superior than 90 %. The mechanism of sorption was studied applying well known kinetic reaction- and diffusion-based models.

[P-EE48]

Design of experiments and response surface methodology as powerful tools for optimization of adsorption heat pumps

J.M. Pinheiro[1], *S. Salústio*[2], *A.A. Valente*[1], *C.M. Silva*[1,*]
[1] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;*
[2]*Department of R&D of Bosch Thermotechnology, Cacia-Aveiro 3800-533, Portugal.*
**carlos.manuel@ua.pt*

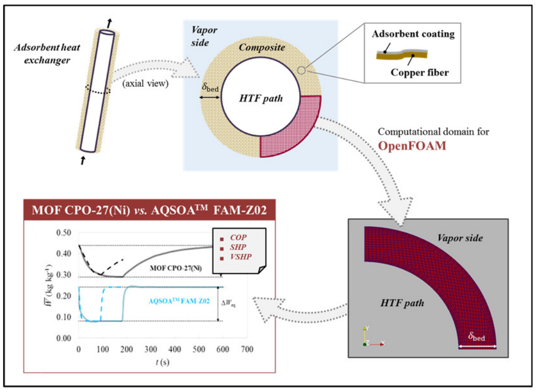


The performance of commercial binderless and binder-containing 13X and NaY for water adsorption heat pumps (AHPs) was compared in this work. Accounting for a Box-Behnken design with four factors (condensation temperature; heat source temperature; time of adsorption and desorption; bed thickness) and three levels, a set of 25 simulations per adsorbent was accomplished, and the performance of the AHPs was evaluated by means of the coefficient of performance (*COP*) and the specific heating power (*SHP*). The results suggested that the presence of the binder in the formulation of 13X does not penalize the zeolite performance significantly, and that the binderless NaY is the most promising material. For the latter adsorbent, statistical outcomes were analyzed and insights about their usefulness to optimize the design and operation of AHPs are provided. Pareto charts displaying the impact ranking of the factors upon *COP* and *SHP* are discussed, and simple equations for the expeditious estimation of both indicators are provided. Such models were used to map the system performance and to select optimal geometric/operating parameters that meet specific performance requisites.

[P-EE49]

Copper foam coated with CPO-27(Ni) metal-organic framework for adsorption heat pump: Simulation study using OpenFOAM

J.M. Pinheiro[1], S. Salústio[2], V. Geraldes[3,], A.A. Valente[1], C.M. Silva[1,**]*
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal; [2] Department of R&D of Bosch Thermotechnology, Cacia-Aveiro 3800-533, Portugal; [3] Center of Physics and Engineering of Advanced Materials, University of Lisbon, 1049-001 Lisboa, Portugal.
** vitor.geraldes@tecnico.ulisboa.pt; **carlos.manuel@ua.pt*

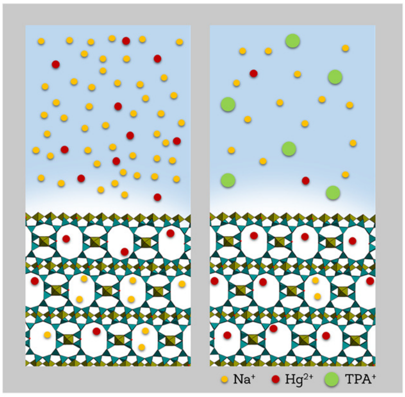


The performance of the metal-organic framework (MOF) CPO-27(Ni) for adsorption heat pumps (AHPs) using water as adsorbate was investigated in this work through modeling and CFD simulations. A customized solver and methodology for simulating adsorption cycles were developed in OpenFOAM and then validated with literature data. Due to the potential of adsorbent coatings and metal fibers and foams for improving AHPs performance, a tube surrounded by a composite of copper foam and CPO-27(Ni) coating was considered. The AHP performance was evaluated through the coefficient of performance (*COP*) and the specific heating power (*SHP*). The obtained COPs and SHPs for the composite coating CPO-27(Ni)/copper foam were 1.16-1.39 and 1922-5130 W kg^{-1}. Under similar conditions, the MOF performance was outperformed by the well-known adsorbent AQSOA™ FAM-Z02, essentially due to the faster intraparticle mass transfer kinetics of the benchmark material.

[P-EE50]

Influence of distinct cations in solution on the equilibrium and kinetics of mercury removal using titanosilicate ETS-4

S.P. Cardoso[1,], T. Faria[1], C.B. Lopes[1], E. Pereira[2], I. Portugal[1], C.M. Silva[1]*
[1]CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus de Santiago 3810-193, Aveiro, Portugal; [2] CESAM, Department of Chemistry, University of Aveiro, Campus de Santiago 3810-193, Aveiro, Portugal.
** simaocardoso@ua.pt*



The removal of Hg^{2+} from aqueous solution was studied by ion exchange with titanosilicate ETS-4. Isothermal batch experiments were carried out using different alkaline solutions for pH adjustment in order to investigate the influence of cation size upon ion exchange equilibrium and kinetics. TPAOH and NaOH were selected as TPA^+ cannot penetrate ETS-4 pores, while Na^+ diffuses through the solid. The results showed that ETS-4 is highly effective for Hg^{2+} removal and that cation size has no impact on equilibrium but it influences the ion exchange kinetics, which is faster when TPAOH is utilized instead of NaOH.The equilibrium of Hg^{2+}/Na^+/ETS-4 systems was accurately modeled by mass action law written in terms of activities. The Maxwell-Stefan (MS) approach was chosen to model the removal kinetics and was able to represent experimental data successfully with a small average deviation (5.81 %).

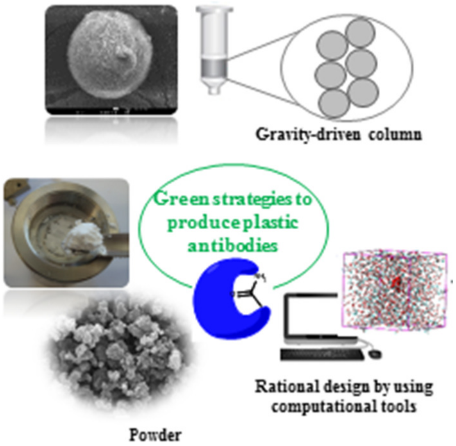
Poster Session

INNOVATIVE MATERIALS AND APPLICATIONS

[P-IM01]

Green and sustainable strategy to produce plastic antibodies for highly-specific pharma separation processes

*R. Viveiros, T. Casimiro**
[1]*CleanMIPTech group, LAQV-REQUIMTE, Chemistry department, Faculty of Sciences and Technology, NOVA University of Lisbon, 2829-516 Caparica, Portugal.*
** teresa.casimiro@fct.unl.pt*

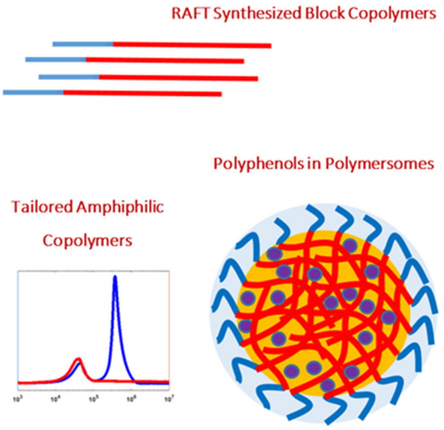


Pharmaceutical industry spends between 50 to 80 % of production costs in API (Active Pharmaceutic Ingredients) purification processes. To address this worldwide demand, several highly-specific separation processes/materials have been proposed, such as plastic antibodies. The use of the Green Chemistry principles has changed the way materials are produced. Green technologies applied on the development of plastic antibodies [1] are appearing not only due to environmental issues but also by the improved features of the final product and process itself. Plastic antibodies have been developed in our lab using supercritical carbon dioxide ($scCO_2$) technology for a wide range of applications, such as API purification [2], enrichment of natural products [3], removal of contaminants from diesel [4] and from water resources [5]. The plastic antibodies are typically obtained as solvent-free, ready-to-use and easy-to-handle dry-powders with narrow particle size distribution.

[P-IM02]

Design of RAFT synthesized amphiphilic and stimuli-responsive block copolymers for encapsulation of polyphenols in polymersomes

C.P. Gomes[1], R.C.S. Dias[1,], M.R.P.F.N. Costa[2]*
[1] *LSRE and Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal;* [2] *LSRE-Faculdade de Engenharia da Universidade do Porto, Rua Roberto Frias s/n, 4200-465 Porto, Portugal.*
** rdias@ipb.pt*

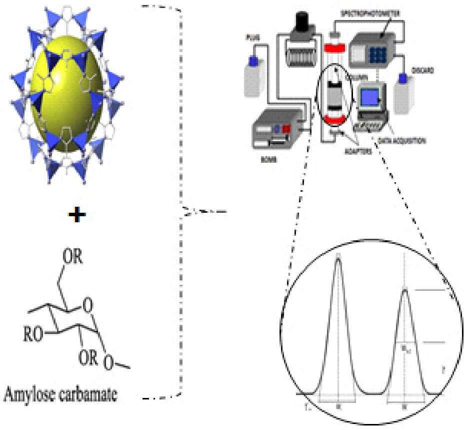


This research is devoted to the design and synthesis of amphiphilic/stimuli-responsive block copolymers for encapsulation of polyphenols in polymersomes. The Reversible Addition-Fragmentation Chain Transfer (RAFT) polymerization technique is used to get tailored amphiphilic block copolymers. Multiple combinations between hydrophilic/hydrophobic monomers, RAFT agents and initial compositions are the main design variables of the synthesis runs. Experimental studies are guided by modeling tools to aid in the design of the materials (e.g. to specify the sizes of the two blocks, pH sensitivity). Isolated polyphenols (e.g. resveratrol, quercetin) and more complex extracts from different kinds of plants are afterwards encapsulated in polymersomes, aiming at the development of carriers for protection and controlled release of these bioactive compounds. It is shown that the produced aggregates have a long colloidal stability and are promising vehicles for the stimulated-release of polyphenols.

[P-IM03]

Adsorbent based on ZIF-8 for chiral separations in liquid chromatography

T.R. Menezes[12], *J.F. de Conto*[12], *S.M. Egues*[2], *C.C. Santana*[1]*.
[1] *Nucleus of Studies in Colloidal Systems (NUESC), Tiradentes University – UNIT, Av. Murilo Dantas, 300, CEP-490032-490, Aracaju-SE, Brazil.*; [2]*Synthesis Materials and Chromatography Laboratory – LSINCROM, Tiradentes University – UNIT, Av. Murilo Dantas, 300, CEP-490032-490, Aracaju-SE, Brazil.*
* *cesarcsantana@gmail.com*

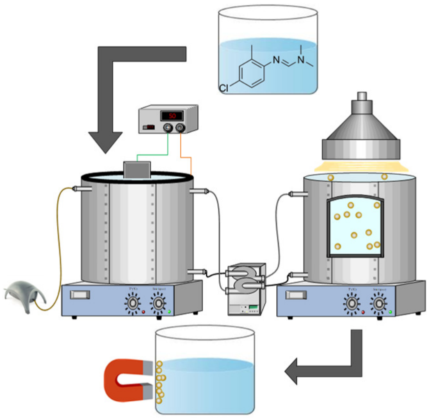


The pharmaceutical industry has shown a special interest on chiral separations exhibiting high financial investment in studies of new chiral stationary phases (CSPs) aiming at high capacities and selectivities. In nowadays the commercial CSPs are mainly based in polysaccharides supported in silica. In this scenery the metal organic frameworks (MOFs) has gained importance due to his high porosities and multiple active sites as promising new stationary phases for liquid phase chromatography (HPLC). Metal organic belongs to a class of coordination polymers than can be used as micro and mesoporous materials of high adsorption capacity. This crystalline tri-dimensional structure combines organic parts with metals forming covalent bonds. Other important class of MOFs exhibit outstanding interest with a combination of high thermal stability and are named zeolite imidazole frameworks (ZIFs) as they use crystalline porous frameworks formed by methalic ions linked to a main imidazole structure.

[P-IM04]

Sequential photocatalysis-electro-Fenton process mediated with magnetic Fe-TiO$_2$ beads for the treatment of polluted effluents

S. Rezgui[1,2], *A.M Díez*[1,]*, *M. Pazos*[1], *M. A. Sanromán*[1], *L. Monser*[2], *N. Adhoum*[2].
[1] *Bioengineering and sustainable research group, University of Vigo, Spain;* [2] *Research Unit in Electrochemistry, Materials and Environment, University of Kairouan, Tunisia.*
* *adiez@uvigo.es*

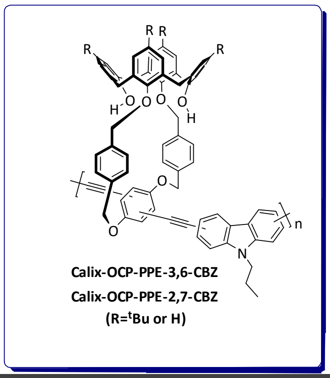


Advanced oxidation processes are widely known for being an alternative for treating effluents polluted with stable compounds such as the pesticide Chlordimeform. The photo-electro-Fenton process is among the most powerful ones. However, the photo-radiation application is a cost which can be justified if enhancing the photo-degradation by adding a photocatalyst. This article is centered on the synthesis of a bifunctional catalyst Fe:TiO$_2$, thus Fe can act as Fenton catalyst and TiO$_2$ a photocatalyst, leveraging the LED radiation applied. Both catalysts were trapped in chitosan beads and synthetized with magnetic properties which would favor their reutilization. A cyclic reactor was set up in order to apply independently and more efficiently the processes. Several variables were optimized and under the optimal conditions, a real wastewater effluent was complete remediated. The catalyst shown an unprecedented stability which demonstrates the good performance of the proposed configuration.

[P-IM05]

Calix[4]arene-carbazole-containing polymers synthesis, properties and thin film as molecular sensors

A.I. Costa[1,2]*, P.D. Barata[1,2], C.B. Fialho[1], J.V. Prata[1,2]
[1] Laboratório de Química Orgânica, Área Departamental de Engenharia Química, ISEL, IPL, R. Conselheiro Emídio Navarro, 1, 1959-007, Lisboa, Portugal; [2] Centro de Química-Vila Real, Universidade de Trás-os-Montes e Alto Douro, 5001-801, Vila Real, Portugal.
*acosta@deq.isel.ipl.pt.



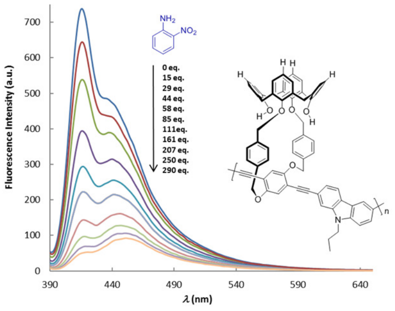
Calix-OCP-PPE-3,6-CBZ
Calix-OCP-PPE-2,7-CBZ
(R=^{t}Bu or H)

Highly fluorescent polymers (CALIX-OCP-PPE-CBZs) were synthesized by Sonogashira-Hagihara cross-coupling polymerizations in good yields using 1,3-oxacyclophane tethered calix[4]arene derivatives integrating carbazole segments as fluorescent signaling moieties. The new materials were characterized by GPC, FT-IR and ^{1}HNMR and their photophysical properties studied by UV-Vis and fluorescence spectroscopies. These new conjugated polymers were used as solid-state fluorescent chemical sensors for the detection of nitroanilines (NAs). Using fluorescence as the transduction technique, experiments have shown that films obtained by drop-coating are selective for *o*-nitroaniline (*o*-NA) as compared with isomeric NAs (*m*-nitroaniline (*m*-NA) and *p*-nitroaniline (*p*-NA)).

[P-IM06]

New bicycle fluorescente calix[4]arene-polymers for molecular sensing in fluid phase

P.D. Barata[1,2]*, A.I. Costa[1,2], C.B. Fialho[1], J.V. Prata[1,2]
[1] Laboratório de Química Orgânica, Área Departamental de Engenharia Química, ISEL, IPL, R. Conselheiro Emídio Navarro, 1, 1959-007, Lisboa, Portugal; [2] Centro de Química-Vila Real, Universidade de Trás-os-Montes e Alto Douro, 5001-801, Vila Real, Portugal.
*pbarata@deq.isel.ipl.pt

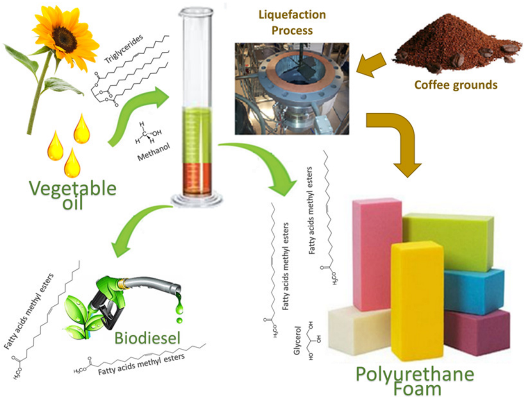


The potential of new fluorescent polymers (CALIX-OCP-PPE-CBZs) toward the selective detection of isomeric nitroanilines (NAs) and explosives, namely 2,4,6-trinitrotoluene (TNT) and picric acid (PA) was evaluated in fluid phase. All polymers showed a considerable photoluminescence (quantum yields ranging from 0.44 to 0.65 in $CHCl_3$) and a great stability toward photobleaching. A Stern-Volmer analysis of steady-state fluorescence data in solution showed that all polymers display a better response and a differentiated sensitivity for NAs than for explosives. In particular, a remarkable response for *o*-NA was retrieved, as could be evaluated from the corrected Stern-Volmer constants (K_{sv} up to 1.3×10^4 M^{-1} in $CHCl_3$).

[P-IM07]

Functional bio-based polyurethane foams from industrial residues

N.V. Gama [1,*], *A. Ferreira* [2], *A. Timmons* [1]
[1] *CICECO - Aveiro Institute of Materials and Department of Chemistry, University of Aveiro – Campus Santiago, Aveiro, Portugal;* [2] *Escola Superior de Tecnologia e Gestão de Águeda - Rua Comandante Pinho e Freitas, Águeda, Portugal.*
** nuno.gama@ua.pt*

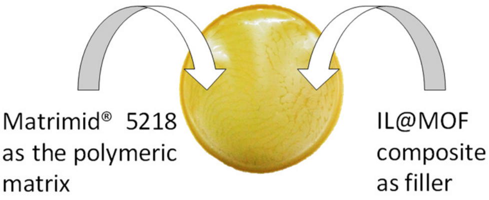


In view of the dependence of the polyurethane foams (PUFs) industry on fossil resources, crude glycerol (CG) a byproduct of biodiesel industry was used as the polyol component in the production of PUFs. The effect of CG composition as well as the effect of the reactants used in PUFs formulations on PUFs properties was studied. From the results it was observed that density and thermal conductivity are governed by the blowing agent and surfactant contents, while the mechanical properties are governed by the content of isocyanate and catalyst. As regards the preparation of new functional materials with higher added value, formulations have been developed aiming at materials for enhanced thermal comfort, improved reaction to fire and sound insulation. Finally, a method for recycling PUFs was developed and the product obtained was used as a partial substituent of GC in the production of foams, which have similar properties to the original ones, proving the suitability of the method.

[P-IM08]

Incorporation of IL@ZIF-8 composites into Matrimid® 5218 to produce mixed-matrix membranes for gas separation

T.J. Ferreira [1], *B.Q.C.A. Moura* [1], *L.A. Neves* [1], *J.M.S.S. Esperança* [1,*], *I.A.A. C. Esteves* [1,*]
[1] *LAQV/REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, Caparica 2829-516, Portugal*
** iaesteves@fct.unl.pt ; jmesp@fct.unl.pt*

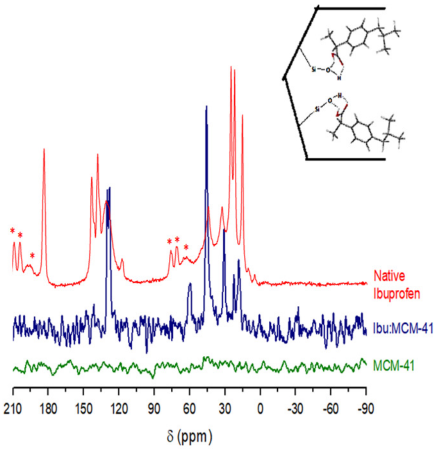


Low-energy demanding, environmentally friendly and cost-effective strategies to mitigate greenhouse gas (GHG) emission to the atmosphere are vital and expected. Metal-Organic Frameworks (MOFs) and Ionic Liquids (ILs) stand out as promising alternatives to more traditional materials for gas separation, mainly due to their high CO_2 sorption and their physicochemical properties. Their combination into IL@MOF composites have potential to improve gas uptake or/and selectivity in adsorption-based processes. Also, the use of mixed-matrix membranes (MMMs) combining a polymeric matrix with a filler is a potential alternative process for CO_2 separation. High CO_2 permeability, chemical and thermal resistances can arise when using MOFs fillers. This solves the trade-off problem of polymeric membranes by combining the sieving effect of MOFs with the properties of polymeric matrixes. Moreover, the use of IL@MOF composites as fillers in MMMs have shown advantages on their mechanical properties and gas permeability and/or selectivity.In this work, IL@MOF composites, previously developed, were used as fillers in a Matrimid® 5218 matrix. The performance study of the MMMs produced is ongoing to assess their CO_2/CH_4 separation ability.

[P-IM09]

Chemical-physical study of ibuprofen incorporated into unmodified and modified mesoporous silicas: From matrix synthesis to drug release

S. Inocêncio[1], I. Matos[1], F. Danède[2], A.F.M. Santos[1], J.C. Sotomayor[1], I.M. Fonseca[1], N.T. Correia[2], M. Dionísio[1], M.C. Corvo[3], T. Cordeiro[1]*
[1]LAQV-REQUIMTE/CQFB, Dep. Química, Fac. Ciências e Tecnologia – UNL, 2829-516 Caparica, Portugal; [2]Univ. Lille, CNRS, UMR 8207, UMET, Unité Matériaux et Transformations, F-59000 Lille, France; [3] i3N|Cenimat, Dep. Ciência dos Materiais, Fac. Ciências e Tecnologia – UNL, 2829-516 Caparica, Portugal.
**tmc18031@campus.fct.unl.pt*

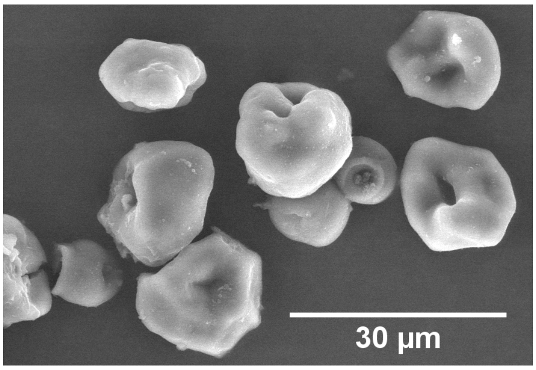


Aiming to stabilize Ibuprofen (Ibu) in the amorphous form, it was loaded by capillarity in MCM-41 and modified MCM-41$_{syl}$. The obtained composites were characterized by ATR-FTIR, ssNMR, DSC and TGA. The thermal decomposition occurs at a higher temperature relative to Ibu, indicating an increase of thermal resistance of the drug in both matrices; the decomposition occurs in a two-step profile, pointing to two different populations (bulk-like and another which interact with the pore surface). The calorimetric detection of a glass transition and the absence of melting confirmed the amorphization of Ibu in the composites. Moreover, the DSC thermograms evidence a bimodal heat flux discontinuity and a shift of the glass transition temperature to higher temperatures more significant in MCM-41$_{syl}$ due to stronger interactions of the drug with the host surface. The drug release studies were carried out in a PBS buffer (pH=6.8), analyzed with UV-VIS and simulated with several kinetic models.

[P-IM10]

Crosslinked starch/chitosan microparticles as reinforcement of thermoplastic corn starch

D. Paiva [1], A.M. Pereira [2], A.L. Pires [2], J. Martins [1,3], L.H. Carvalho[1,3], F.D. Magalhães [1]*
[1]LEPABE, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal; [2]IFIMUP and IN – Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, 4169-007 Porto, Portugal; [3]DEMad - Instituto Politécnico de Viseu, Campus Politécnico de Repeses 3504-510, Viseu, Portugal.
**lhcarvalho@estv.ipv.pt*

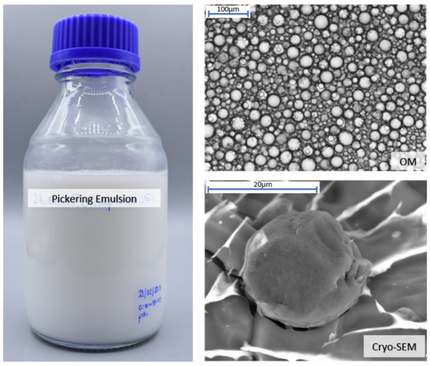


Thermoplastic corn starch (TPS) materials are known to have limitations regarding their application as biodegradable material for short lifetime products. This study proposes the incorporation of starch/chitosan microparticles crosslinked with glutaraldehyde (SCM) in a TPS matrix plasticized with glycerol. The use of microparticles made of starch increase the compatibility with the TPS matrix. Morphological, thermal and water solubility and boiling water solubility were conducted on the SCM particles to assess their stability in different conditions. X-ray diffraction performed to the SCM indicated that crosslinked starch avoids retrogradation. Tensile strength, Young's modulus and toughness were improved with the incorporation of 30 % (w/w) of SCM in the TPS. The elongation of these materials was also improved. A slight decrease in the water uptake was detected when SCM was incorporated in the matrix.

[P-IM12]

Novel O/W green emulsions stabilized with nano-hydroxyapatite solid particles – Pickering emulsions

A. Ribeiro[1,2,3,*], *Y.A. Manrique*[1], *I.C.F.R. Ferreira*[2], *M.F. Barreiro*[3], *J.C.B. Lopes*[1], *M.M. Dias*[1]
[1] *Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials, Rua Roberto Frias, Porto, Portugal;* [2] *Mountain Research Center, Campus Santa Apolónia, Bragança, Portugal;* [3] *Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials, Campus Santa Apolónia, Bragança, Portugal.*
**asribeiro@fe.up.pt*

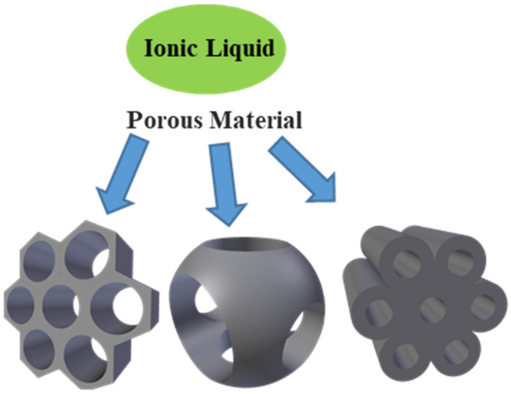


Surfactant-free emulsions have been gaining increasing interest along the last years. In this context, Pickering emulsions, characterized by using solid particles as stabilizers provide an innovative, promising and green alternative to produce stable emulsions. In this work, Pickering emulsions were developed using sunflower oil dispersed in water and stabilized with nano-hydroxyapatite (n-HAp). The impact of nanoparticle's concentration, and oil-water ratio were studied on the emulsion stability and type. Stability, droplet's size and morphology were monitored during storage time by optical microscopy (OM), and cryo-scanning electron microscopy (Cryo-SEM). The presence of n-HAp at the oil-water interface was confirmed by both techniques. A model was developed to predict the stability behaviour of Pickering emulsions based on the distance between the n-HAp particles that remain free in solution.

[P-IM13]

Sorption of fluorinated greenhouse gases using fluorinated ionic liquids

J.E. Sosa[1], *R.P.P.L. Ribeiro*[1], *J.P.B. Mota*[1], *J.M.M. Araújo*[1], *A.B. Pereiro*[1]
[1]*LAQV, REQUIMTE, Department of Chemistry, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal.*
** anab@fct.unl.pt*

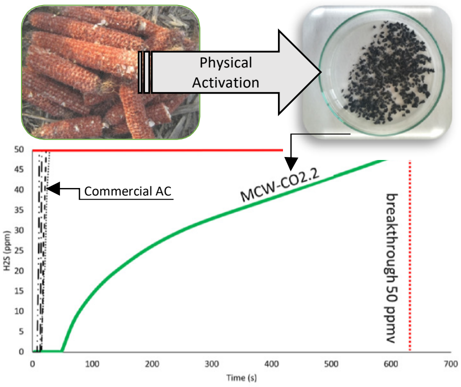


The production of fluorinated gases has drastically increased in recent years as a consequence of the need to replace ozone-depleting substances that phased out under the Montreal's Protocol. Fluorinated gases are a good solution as they are very energy efficient, ozone-friendly and safe for users, with low levels of flammability and toxicity. However, some of these compounds have a large global warming potential, and their emissions to the atmosphere should be considerably reduced according to the Kyoto's protocol and the new European Union (EU) regulation (No 517/2014). In order to reduce these emissions, different climate-friendly and safe solvents are under development. However, there is no "one size fits all" solution: the usefulness and suitability of each solvent must be considered separately for each product, equipment and industrial process. The main objective of this work is to study alternative solvents environmentally benign and more energy efficient for the recycling/recovery of the fluorinated gases. With this goal in mind, fluorinated ionic liquids were supported on a porous material and isotherms of different fluorinated greenhouse gases were determined.

[P-IM14]

New eco-sorbents for hydrogen sulphide removal from biogas

E. Surra[1], M. Nogueira[1], M. Bernardo[2], I. Fonseca[2], I.A.A.C. Esteves[2] , N. Lapa[1*]
[1] LAQV-REQUIMTE, Departamento de Ciências e Tecnologia da Biomassa; [2] LAQV-REQUIMTE, Departamento de Química; Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal.
*ncsn@fct.unl.pt

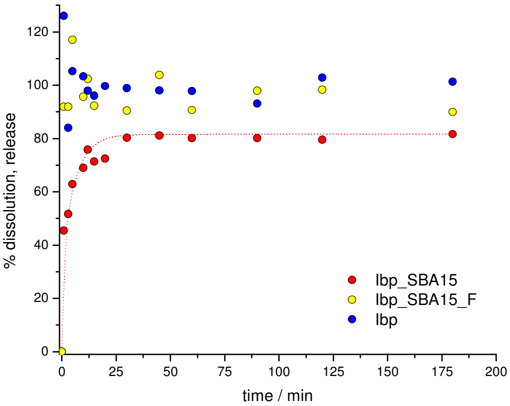


The H_2S removal capacity from a real biogas stream by activated carbons (AC) produced from Maize Cob Waste (MCW) was tested. The AC samples were produced by both activation with CO_2 and functionalisation with a by-product of anaerobic digestion - Liquid Digestate. The physical activated carbon (MCW-CO2.2) provided the highest H_2S removal capacity with a value of 15.1 mg H_2S/g due to its better textural properties and probable presence of oxygen active sites that favoured the catalytic oxidation of H_2S on the AC surface; this AC can be considered an interesting adsorbent for H_2S removal from a real biogas stream at the conditions currently applied in industrial plants.

[P-IM15]

Influence of the treatment of mesoporous silica surfaces in the release profile of a loaded drug

R. Domingos[1], T. Cordeiro[1], I. Matos[1], J.C. Sotomayor[1], I.M. Fonseca[1], M.M. Cardoso[1], M. Dionísio[1], M.T. Viciosa*[2]
1LAQV-REQUIMTE/CQFB, Dep. Química, Fac. Ciências e Tecnologia – UNL, 2829-516 Caparica, Portugal; 2 CQFM, Centro de Química-Física Molecular, IN—Institute of Nanosciences and Nanotechnology, Instituto Superior Técnico,1049-001 Lisboa, Portugal.
* teresaviciosa@ist.utl.pt

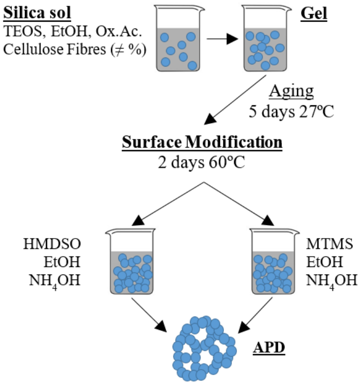


The present work aims to obtain a drug delivery system using mesoporous silica as carrier to stabilize ibuprofen (IBP) drug in the amorphous state. Two mesoporous silica matrixes (SBA-15): unmodified and methyl-functionalized were used with pore diameters of 6.8 and 6.7 nm, respectively. The amount of drug loaded was quantified by thermogravimetric analysis being 90% (v/v). Differential scanning calorimetry (DSC) and ATR-FTIR spectroscopy gave evidence of successful IBP incorporation in the matrices. The glass transition of IBP was detected by DSC showing that the drug is in the amorphous state; however a small fraction remains crystalline outside pores. The mobility studied by Dielectric Relaxation Spectroscopy of IBP inside pores was found much slower than that of bulk IBP. Drug delivery was monitored by UV-VIS spectroscopy showing: a) all the incorporated drug is released and b) it is faster from the functionalized silica due to suppression of guest-host hydrogen bonding.

[P-IM16]

Silica aerogel reinforcement with different types of cellulose fibres

A. Romeiro[1], L. Durães[1], A. Portugal[1,]*
[1] CIEPQPF, Chemical Engineering Department, University of Coimbra, 3030-790 Coimbra, Portugal
** atp@eq.uc.pt*

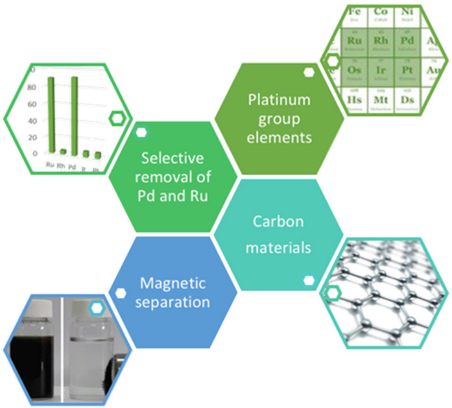


Four different type of cellulose fibres were used, namely raw pasta of eucalyptus, raw pulp of sodra (pine + spruce), white eucalyptus pulp and white sodra pulp. The influence of the amount and quality of fibres in the gelation time, density and monolithic nature of the aerogels has been assessed. In this study, we have obtained different results when we used TEOS or TMOS precursor for the density and shrinkage.

[P-IM17]

Selective recovery of platinum-group elements using Fe_3O_4@EG nanocomposites and their precursors

*F. Rocha[1 *], E. Pereira[2], T. Trindade[1], C.M. Silva[1], C.B. Lopes[1]*
[1] Universidade de Aveiro and CICECO, Aveiro, Portugal; [2] Universidade de Aveiro and CESAM, Aveiro.
** filipe.rocha@ua.pt*

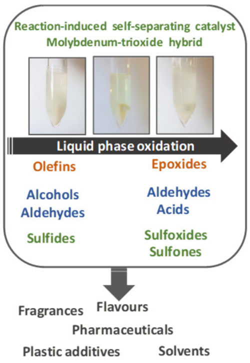


The Platinum-group elements (PGE) consists in six precious metallic elements (Ru, Rh, Pd, Os, Ir and Pt), that due to their unique characteristics are widely used in many applications. More, due to their economic importance it is crucial to recycle these elements, and their recovery from solutions it is an important step on that process. In this work, two magnetic composites had been synthesized using exfoliated graphite and magnetite nanoparticles as precursors. Afterwards, all materials have been investigated as sorbents for PGE removal, by carrying out batch experiments. Characterization results proved that composites were successfully synthetized and have different amounts of magnetite. Removal efficiency results have revealed a high dependency from pH and sorbent material for Pt, Ir and Rh. Pd and Ru had similar results, with the greatest removal efficiencies (~90%). The application of these composites for PGE removal constitutes a promising step in the recycling of some PGE.

[P-IM18]

A new molybdenum trioxide hybrid decorated by 3-(1,2,4-Triazol-4-yl)adamantane-1-carboxylic acid: A promising reaction-induced self-separating catalyst for epoxidation

P. Neves[1,*], *A.B. Lysenko*[2], *G.A. Senchyk* [2], *K.V. Domasevitch*[2], *H. Krautscheid*[3], *A.A. Valente*[1], *I.S. Gonçalves*[1]
[1] *Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal;* [2] *Inorganic Chemistry Department, Taras Shevchenko National University of Kyiv, Volodimirska Str. 64, Kyiv 01033, Ukraine;*[3] *Institut für Anorganische Chemie, Universität Leipzig, Johannisallee 29, D-04103 Leipzig, Germany.*
** pneves@ua.pt*

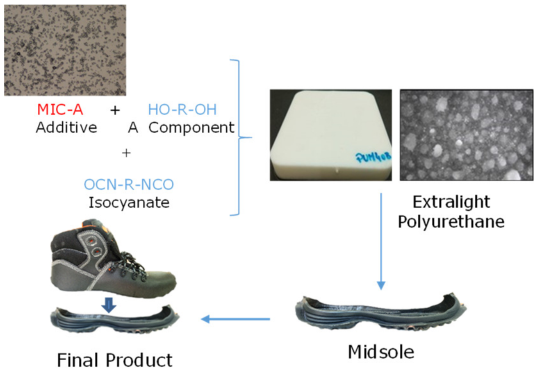


A new 1D Mo-trioxide hybrid, $[MoO_3(\mathit{tradc}H)]\cdot H_2O$ (**1**) was synthesized by treatment of the heterobifunctional organic ligand 3-(1,2,4-triazol-4-yl)adamantane-1-carboxylic acid (*tradc*H) with MoO_3 under hydrothermal conditions. Compound **1** is a rare case of a hybrid compound that acts as a reaction-induced self-separating (RI-SS) catalyst using hydrogen peroxide as eco-friendly oxidant that gives water as co-product. The original solid material converts into soluble active species, and the latter revert to the original material after the consumption of the oxidant, precipitating and allowing ease of catalyst separation/reuse (in a similar fashion to heterogeneous catalysts). This compound was explored for a chemical reactions scope covering sulfoxidation, alcohol oxidative dehydrogenation, aldehyde oxidation, and olefin epoxidation.

[P-IM19]

Ultralight microcellular polyurethanes for the production of technical footwear components

H. Rafael[1], *I.P. Fernandes*[1], *H.T. Gomes*[1], *V. Pinto*[2], *A.M. Fernandes*[3], *M.J. Ferreira*[2], *M.F. Barreiro*[1]
[1]*Mountain Research Centre (CIMO) and Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (LSRE-LCM), Polytechnic Institute of Bragança, Campus de Santa Apolonia - 5300-253 Bragança, Portugal*
[2]*Centro Tecnológico do Calçado de Portugal (CTCP), Rua de Fundões - Devesa Velha, 3700-121 S. João da Madeira, Portugal,*
[3]*AMF Lda, Rua São Cipriano nº 658 Tabuadelo, 4835-461 Guimarães, Portugal.*
** barreiro@ipb.pt*

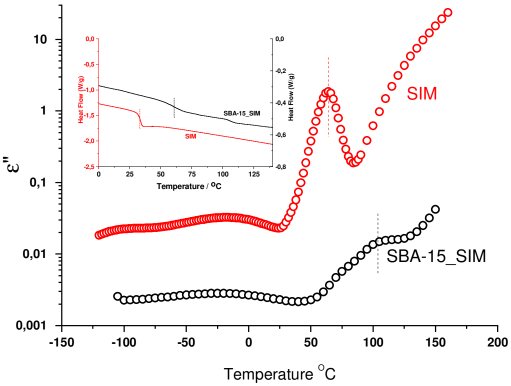


Today's society demands lightweight and comfortable footwear products, which represents a market opportunity for the footwear industry, motivating the development of new low-density (ultralight) materials. This research is dedicated to the development of ultralight microcellular polyurethanes (PUs) with suitable properties for the production of midsoles for technical footwear. In this context, the studies performed in this work aimed at reduce the density of microcellular PUs by the incorporation of additives based on expandable thermoplastic microspheres. Samples of a base formulation were modified by the incorporation of 1, 2 and 3% of the additive. The produced materials result in PUs with densities that varied from 0.45 to 0.30 g/cm^3. The performed characterization pointed out for PUs with adequate technical properties, with particular emphasis for impact absorption, which evidenced the suitability of the developed materials for the production of midsoles for ultralight safety shoes.

[P-IM20]

Stabilizing simvastatin in the amorphous state into nanostructured matrices

A. Franco[1], *T. Cordeiro*[1], *I. Matos*[1], *C.V. Pereira*[2], *J.C. Sotomayor*[1], *I.M. Fonseca*[1], *M.M. Cardoso*[1], *A. Matias*[2], *M. Dionísio*[1], *M.T. Viciosa*[*3]
[1] *LAQV-REQUIMTE/CQFB, Dep. Química, Fac. Ciências e Tecnologia – UNL, 2829-516 Caparica, Portugal;* [2] *Nutraceuticals and Bioactives Process Technology, iBET - Instituto de Biologia Experimental e Tecnológica, Oeiras, Portugal;* [3] *CQFM-IN, Instituto Superior Técnico,Universidade de Lisboa, 1049-001 Lisboa, Portugal.*
** teresaviciosa@ist.utl.pt*

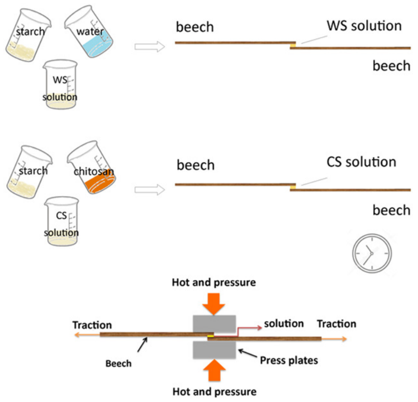


The modification of a drug's physical state is a promissory route to turn it more soluble. In this work, a drug delivery system was prepared to improve simvastatin (SIM) solubility taking advantage of the amorphous state. SIM was incorporated in SBA-15 mesoporous matrices unmodified and functionalized by methylation both with pore size (~6.7nm). Attenuated total reflectance, NMR and TGA evidence efficient inclusion in matrices. A loading of 49%(w/w) in the composite was determined corresponding to a pore filling of 98%(v/v). In SBA-15_SIM, a glass transition (Tg) is detected at 59oC showing that the incorporated drug is in the amorphous state, however with an increased Tg (Tg, CIM = 30 ºC). The mobility hindrance inside pores is confirmed by Dielectric Relaxation Spectroscopy. Cytotoxicity essays show as at higher concentrations SIM is less cytotoxic when in composite. Release essays followed by UV-VIS spectroscopy suggest a faster release from the unmodified silica.

[P-IM21]

Use of ABES to evaluate the impact of chitosan solution on the cure of starch based resins

M.L. Almeida[1,*], *J.M. Martins*[2], *C. Coelho*[2], *F.M. Magalhães*[1], *L.H. Carvalho*[2]
[1]*LEPABE, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, 4200-465, Porto, Portugal;*
[2]*DEMad - Escola Superior de Tecnologia e Gestão de Viseu, Campus Politécnico, 3504-510, Viseu, Portugal.*
**malmeida@fe.up.pt*



In the last years, due to the increasing environmental awareness, sustainable solutions are being sought for the use of composites produced from renewable materials, such as wood and other lignocellulosic materials, as well as natural adhesives. A cheap, eco-friendly polysaccharide found all over the world is starch, which can be used as adhesive in wood composites. A new biobased foamable sour cassava starch resin was developed to be used in particleboard production. This formulation is used chitosan solution as additive, a common crosslinker used in starch resins. The impact of the use of chitosan solution on adhesive performance was studied using ABES (Automated Bonding Evaluation System). This equipment was used to evaluate the cure of the mix starch + chitosan solution, as well the mix of starch + water. The performed tests were all carried out at the same pressing temperature and using the same pressing times.

[P-IM22]

BioFPro a web based software for correlation and prediction of biofuels properties

A. Ferreira[1,*], *N.M. C. Talavera-Prieto*[1,2], *J. Granjo*[1]
[1] *CIEPQPF, Department of Chemical Engineering, University of Coimbra, Polo II, Rua Silvio Lima, 3030-970 Coimbra, Portugal*
[2] *CECOAL-CONICET-UNNE, Ruta 5 Km 2.5, 3400 Corrientes, Argentina;*
* *abel@eq.uc.pt*

Welcome to Biodiesel Properties (BioF Pro) / version 1

BioF Pro is a software designed to the calculation of biofuels thermodynamic properties using an integrated approach. In this approach the theory behind calculation of each of property is available. Prediction, interactivity and development are the base trilogy of these tools.

BioF Pro covers all the important properties of biofuels that influence the engine operation related to the standards in the CEN EN in Europe and ASTM in USA.

BioF Pro uses the Javascript for WEB which brings a lot of flexibility using some important existing plugins and web visualization and calculation resources.

An extensive property database constructed for the different properties of biofuels are given and will be updated.

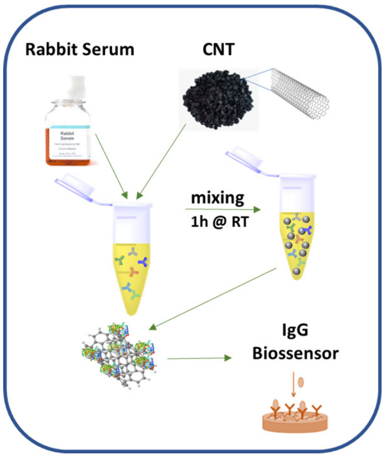
Mail: abel@eq.uc.pt

The need of thermophysical properties in the production, transportation, storage, and combustion of biofuels requires the availability of dedicated software for property prediction. Most of software packages for thermodynamic calculations or in commercial process simulators used in biofuel processing require commercial licenses that may have prohibitive acquisition or maintenance fees. There have been some rare attempts to generate free software in the scope of calculating biofuels thermodynamic properties. In this work, it is presented BioFPro, a new software for the estimation and correlation of biofuels thermophysical properties. Some of them (e.g., density and viscosity) are calculated in wide ranges of temperature and pressure, using different models based on the Principle of Corresponding States, the concept of Contribution of Groups and empirical correlations.

[P-IM23]

Modified carbon nanotubes as alternative platforms for the adsorption of immunoglobulin G

D.F. de Castro[1], *M.C. Neves*[1], *J.A.P. Coutinho*[1], *J.L. Faria*[2], *M.G. Freire*[1], *C.G. Silva*[2]. *A.P.M. Tavares*[1,*]
[1]*CICECO – Aveiro Institute of Materials, Chemistry Department, University of Aveiro, Aveiro, Portugal;* [2]*Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (LSRE-LCM), Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal.*
**danielfcastro@ua.pt ; aptavares@ua.pt*

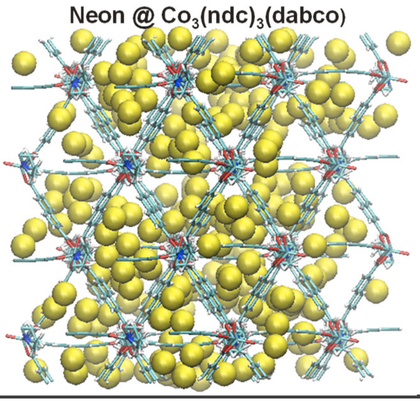


Antibodies (Ab's) are molecules with high specificity for binding and inactivation of antigens, such as bacteria and virus. Ab's, such as immunoglobulin G (IgG), have been the subject of research for the treatment of infectious diseases and as new therapies for cancer. However, Ab's are among the most expensive therapeutic options due to the lack of a cost-effective purification method. Thus, there is an urgent need for new purification methods for the IgG production. The main objective of this work was to determine the best operating conditions for purifying IgG from rabbit serum using pristine and modified carbon nanotubes (CNT). Experimental conditions, such as pH, serum and IgG concentrations were optimized. At the best conditions, IgG with a purity of 51.3% and a recovery yield of 99.9% was obtained.The used CNT were chemically, structurally and morphologically characterized by Brunauer–Emmett–Teller(BET) specific surface areas(S_{BET}) and transmission electronic microscopy (TEM).

[P-IM24]

Neon adsorption on metal-organic frameworks over wide temperature and pressure ranges

J. Barreto[1], M. Xavier[1], R.P.P.L. Ribeiro[2,], D. Martins[3], I.A.A.C. Esteves[2], M. Branco[3], G. Bonfait[1], J.P.B. Mota[2,*]*
[1] LIBPhys-UNL – Department of Physics, Faculty of Science and Technology, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal; [2] LAQV-REQUIMTE, Department of Chemistry, Faculty of Science and Technology, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal; [3] Active Space Technologies S.A., Parque Industrial de Taveiro, Lote 12, 3045-508 Coimbra, Portugal.
** rpp.ribeiro@fct.unl.pt ; pmota@fct.unl.pt*

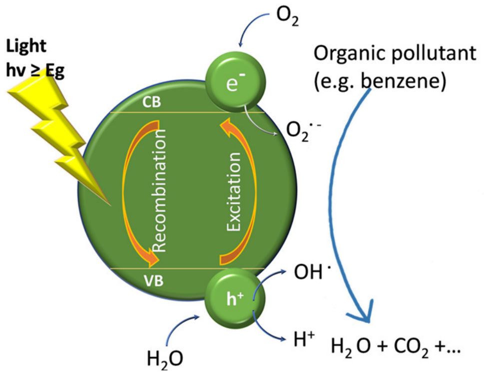


Several metal-organic frameworks (MOFs) were studied with the objective of evaluating their performance for eventual application in adsorption-based coolers. From the huge amount of available MOF structures, a preliminary selection of suitable MOFs was performed through molecular simulation techniques. Three MOFs were selected – HKUST-1, UiO-66, and $Co_3(ndc)_3(dabco)$ – and experimental adsorption equilibria measurements were performed to evaluate the MOFs properties for Neon adsorption. The measurements were performed spanning temperature and pressure ranges of 77 – 500 K and 0 – 100 bar, respectively. The measurement of adsorption equilibria in such broad thermodynamic conditions is not common and the obtained results showed that Neon can be stored in the three MOFs evaluated. The $Co_3(ndc)_3(dabco)$ MOF presents higher adsorption capacity, followed by HKUST-1, and, finally, UiO-66.

[P-IM25]

Titanium oxide-based materials for photo-catalysis of dyes and benzene

M.R.F. Silva,[1,] M.A.O. Lourenço,[1] D.M. Tobaldi,[1] M.P. Seabra,[1] P. Ferreira,[1]*
[1] CICECO – Aveiro Institute of Material, University of Aveiro, 3810-193 Aveiro, Portugal
** mrfs@ua.pt*

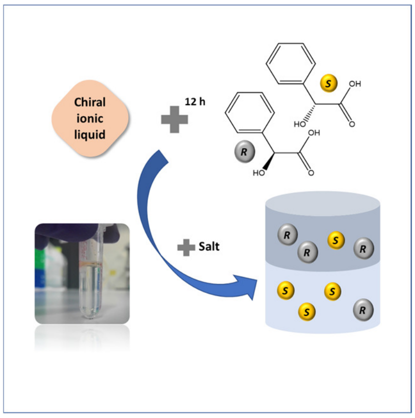


Titanium dioxide (TiO_2), based materials were tested regarding its ability to degrade the dye Rhodamine B (RhB) using UV and visible light, as well as the ability to degrade the volatile organic compound – benzene, using solar light. The pure TiO_2 compounds show a blue shift in the UV-vis analysis of the photodegradation of RhB indicating that photosensitization occurs. This phenomenon was not perceived in samples with added graphene oxide (GO) and carbon nanotubes (CNT). The sample with the highest amount of photosensitization depicted lower photodegradation of benzene than a sample without a blue shift.

[P-IM26]

Enantioselective separation of racemic mandelic acid using aqueous biphasic systems with chiral ionic liquids

M. Kholany[1,*], *F.A. e Silva*[1], *T.E. Sintra*[1], *S.P.M. Ventura*[1], *J.A. P. Coutinho*[1]
[1] *CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal;*
**mariamkholany@ua.pt*

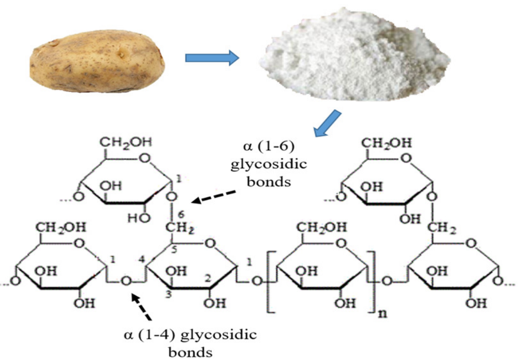


This work proposes the development of a versatile enantioseparation platform for the chiral resolution of racemic mandelic acid (MA). ABS using chiral ionic liquids (CILs) simultaneously as chiral selectors and phase forming agents is proposed. Five ABS were studied to determine the CIL structure and salt role on the ABS aptitude to separate MA enantiomers. Optimization studies were further pursued, as representative CIL-based ABS were employed in optimization studies, where the MA content, temperature, tie-line length, salt and phases weight ratio were studied. The influence of these parameters is shown to be highly dependent on the CIL-based ABS, nevertheless the results attained suggest that the key driving the enantioseparation in these ABS is a combination of the enantiorecognition ability of a given CIL with the solubility of MA in the corresponding CIL-rich phase. By closely manipulating the two conditions of the purification, good enantioselective separations can be achieved.

[P-IM27]

Hydrogen peroxide oxidation of potato Starch

J.V. Barbosa[1,*], *J. Martins*[2], *L. Carvalho*[2], *F.D. Magalhães*[1], *M.M.S.M. Bastos*[1]
[1] *LEPABE—Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;*[2]*DEMAD—Department of Wood Engineering, Polytechnic Institute of Viseu, Campus Politécnico de Repeses, 3504-510 Viseu, Portugal.*
** joanabarbosa@fe.up.pt*

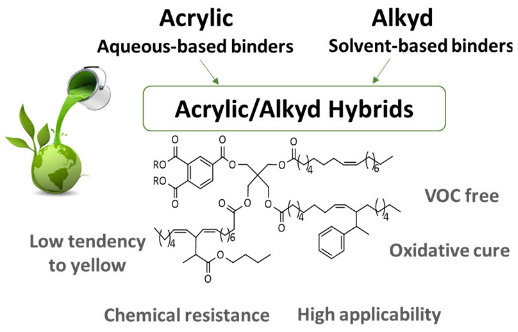


Although starch biodegradable and non-toxicity properties make it an alternative to products based on fossil fuel, its structure and functional properties limits their industrial applications. To overcome these disadvantages chemical, physical or enzymatic modifications can be applied. The present study describes the effect of oxidation reaction with different concentration of hydrogen peroxide (1 and 10 g/kg starch) in potato starch. A gradual increase in carboxyl content with increasing oxidant concentration was observed due to the oxidation of the hydroxyl groups to carboxyl groups. Although SEM analysis showed that the oxidation reaction does not induce changes in the granules morphology, the second derivative FTIR and NMR analyses confirmed the occurrence of oxidation reaction.

[P-IM28]

Development of acrylic/alkyd hybrid polymers

S. Loureiro [1], *J.V. Barbosa* [1*], *J. Moniz*[2], *F.D. Magalhães*[1], *M.M.S.M. Bastos*[1]
[1] *LEPABE - Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;* [2]*Resiquímica – Resinas Químicas, S.A., Rua Francisco Lyon de Castro, 28, 2725-397 Mem Martins, Lisboa.*
** joanabarbosa@fe.up.pt*

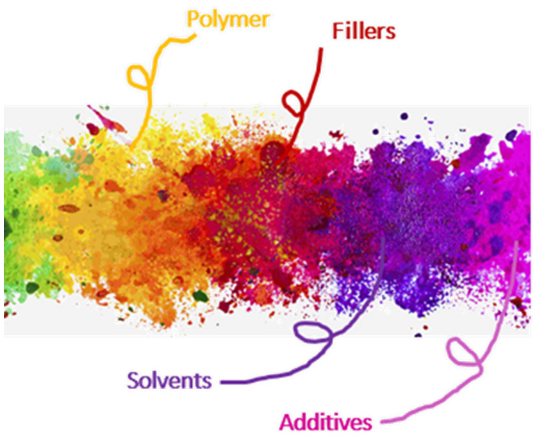


In the present work acrylic/alkyd hybrids were developed to obtain a resin exhibiting properties from both materials, promoting chemical reaction between them and eliminating the presence of organic solvents. Conventional emulsion polymerization and mini-emulsion were used, adding a pre-made alkyd resin (AR) and unsaturated monomers (UM). FTIR and NMR spectrophotometry analyses were used to confirmed chemical reaction between the alkyd resin and the unsaturated monomers. Stable hybrids with 10 % of alkyd resin were produced by mini-emulsion process, when anionic surfactants were used, while colloidal destabilization was observed with conventional emulsion. NMR analyses confirmed the decrease of 67 % of double bounds from the fatty acids of the alkyd resin, suggesting free radical polymerization with the unsaturated monomers.

[P-IM29]

Predicting paint composition from middle infrared spectra (FTIR)

M. J. Fernandes[1], *O. Filipa*[2], *J. Peres* [1], *F. G. Martins* [1], *M.M.S.M. Bastos*[1*]
[1] *LEPABE, Faculdade de Engenharia da Universidade do Porto, s/n, R. Dr. Roberto Frias, 4200-465 Porto, Portugal;*[2] *Barbot Tintas, S.A, R. dos Borneiros 466, 4410-295 Vila Nova de Gaia.*
** mbastos@fe.up.pt*

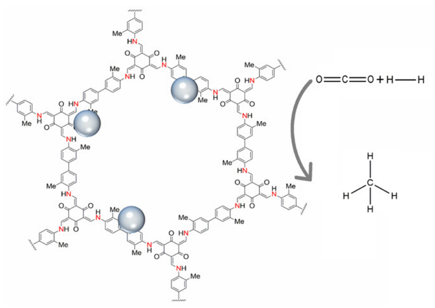


Paints are complex mixtures composed mainly by four constituents: resins, fillers, solvents and additives. Each of these components gives certain characteristics to paints and therefore it is of real importance to identify and quantify them. In this work, FTIR is combined with Partial Least Squares (PLS) regression models. Upon collecting spectral data, models for the quantification of polymer, calcium carbonate, and water content in styrene-acrylic, vinyl and acrylic type paints were developed and evaluated according to some performance indexes for achieving models with good prediction features. Moreover, it was possible to formulate and produce a new paint based on quantified components content of an unknown paint given by the corresponding PLS model. Furthermore, both paints were subjected to quality control tests and the assessed properties were consistent. It can be stated that these PLS models can be used to quality control purposes of paints and for predicting paint composition.

[P-IM30]

Covalent organic frameworks as support for Ni nanocatalysts for CO_2 methanation

L. P. L. Gonçalves [1,2,*], *J. P. S. Sousa* [1], *O. S. G. P. Soares*[2], *Y. V. Kolen'ko*[1], *M. F. R. Pereira*[2]
[1] *International Iberian Nanotechnology Laboratory (INL), Av. Mestre José Veiga s/n, 4715-330 Braga, Portugal;* [2] *Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.*
** liliana.goncalves@inl.int*



CO_2 methanation is a reaction of great interest since it is the most energetically advantageous reaction to valorise CO_2 as carbon source, decreasing the CO_2 emissions to atmosphere. The most used catalysts for this reaction are supported Ni catalysts. The aim of this work was to prepare new and more efficient catalysts for CO_2 methanation by using covalent organic frameworks (COFs) as supports for Ni nanoparticles. We successfully prepared, characterized and tested Ni nanocatalysts over different supports for CO_2 methanation, in order to assess the possibility of using COFs as support for more efficient metal catalysts.

[P-IM31]

Development of new lead-free medical X-ray protective clothing

P.S.F. Ramalho[1, *], *O.S.G P. Soares* [1], *T. V. Pinto* [2], *A.L. Gonçalves*[3], *A. Barros*[3], *G. Santos*[3], *J. Morgado*[3], *C. Freire*[2], *C. Pereira* [2] *and M.F.R. Pereira.*[1]
[1] *Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (LSRE-LCM), Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias s/n 4200-465, Porto, Portugal;* [2]*REQUIMTE/LAQV, Departamento de Química e Bioquímica, Faculdade de Ciências, Rua do Campo Alegre 1021/1055, 4169-007 Porto, Portugal.*
[3]*CentroTecnológico das Indústrias Têxtil e do Vestuário de Portugal (CITEVE), Rua Fernando Mesquita nº 2785, 4760-034 Vila Nova de Famalicão, Portugal.*
** psfr@fe.up.pt.*

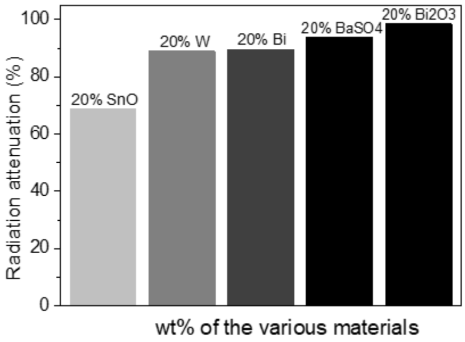


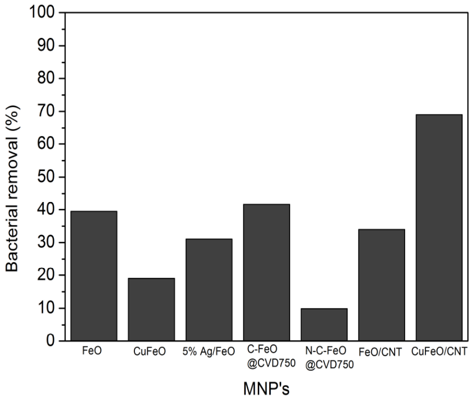
Figure 1. wt% of the metals in the formulation.

Throughout life, humans are daily exposed to the effects of radiation. These radiations can have natural or artificial origins and efforts should be concentrated to reduce their harmful effects. Radiation protection is of fundamental importance is the medical sector, mainly in clinical radiology. As such, all efforts should be directed towards controlling and reducing radiation exposure, and in this context protective clothing plays a key role. The main objective of this work is the development of a lead-free protective clothing with enhanced protection. X-ray attenuation properties were assessed on a set of tissues coated with Bi_2O_3, Bi, W and SnO. A high attenuation of 98 % was obtained for the tissues coated with 20 % of Bi_2O_3.

[P-IM32]

Nanomaterials application in water disinfection for human consumption

A.S.G.G. Santos [1,2]*, P.S.F. Ramalho*[1]*, A.R. Lopes*[2]*, A.G. Gonçalves*[3]*, O.P.C. Nunes*[2]*, M.F.R. Pereira*[1]*, O.S.G.P. Soares*[1]*
[1] *Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials (LSRE-LCM), Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, 4200-465 Porto, Portugal;* [2] *LEPABE - Laboratory for Process Engineering, Environment, Biotechnology and Energy (LEPABE), Departamento de Engenharia Química, Faculdade de Engenharia, da Universidade do Porto, 4200-465 Porto, Portugal;* [3] *Bosch Termotecnologia S.A., EN 16, km 3.7, 3800-533 Cacia, Aveiro, Portugal*
**salome.soares@fe.up.pt.*

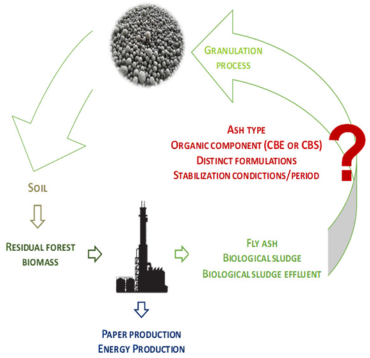


There are innumerous factors associated with the scarcity of drinking water in the world. The achievement of innovative technologies for water treatment becomes crucial in order to guarantee the supply of drinking water and reduce global pollution. Nanomaterials have proven to have great antibacterial action, which make them quite efficient in water disinfection. In this work, eight different magnetic nanoparticles (MNP's) were synthesized, having in their base iron oxides, and were characterized using different techniques. Two different bacteria were used to evaluate the nanoparticles bacterial removal efficiency, *Escherichia coli* (gram-negative) and *Staphylococcus aureus* (gram-positive), respectively. Several tests with different experimental conditions were carried out in a batch reactor. The results showed that the MNP's were efficient in the removal of the two studied bacteria.

[P-IM33]

Valorization of wastes from pulp and paper industry: effect of distinct formulations and stabilization conditions in the properties of granules to be used as soil improvers

N. Cruz[1,*]*, F. Silva*[1]*, L. Tarelho*[2]*, S. Rodrigues*[1]
[1] *University of Aveiro, CESAM & Department of Chemistry, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal;*[2] *University of Aveiro, CESAM & Department of Environment and Planning, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal.*
**nmcc@ua.pt*



Valorization of wastes from pulp and paper industry is necessary to reduce environmental impacts of thermochemical conversion of biomass for heat and power production and to boost the re-use of wastes which otherwise would require landfilling.

The granulation of different waste materials (fly ash, composted biological sludge and biological sludge effluent) proved to be suitable to produce new products that can be used as soil improvers.

Distinct formulations allow us to obtain a wide range of different new products with variable properties (bulk density, organic matter and elemental composition). Stabilization conditions are another key factor in the control of the physical-chemical properties of the materials produced (pH, EC, chloride content and soluble elements).

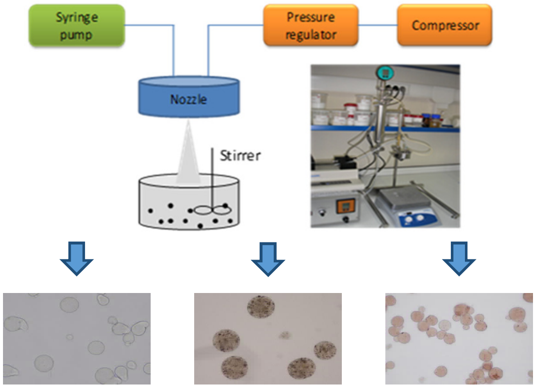
[P-IM35]

Microencapsulation by spray coagulation method: Study of the alginate crosslinking by different calcium salts

D.F. Cuma[1,2], I.P. Fernandes[1,2], M.F. Barreiro[1,2,]*

[1]CIMO, Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal; [2]LSRE-LCM, Polytechnic Institute of Bragança, Campus Santa Apolonia Ap 1134, 5301-857 Bragança, Portugal

**barreiro@ipb.pt*



The use of biopolymers such as alginate has been growing in the last decades due to properties such as non-toxicity and biodegradability. In this work, the microencapsulation of curcumin and safranin, used as model compounds for hydrophobic and hydrophilic active principles, respectively, was studied with alginate matrices by the spray coagulation technique. The alginate ionic crosslinking with three calcium sources (calcium chloride ($CaCl_2$), calcium gluconate and calcium lactate) was considered. The obtained microcapsules were characterized in terms of load, encapsulation efficiency (EE), rehydration capacity, and particle size. The release profiles of both active principles were also studied. Through FTIR analysis the contribution of the calcium source, and the presence of the active principles inside the microcapsules, was identified, while the TGA evidenced an increasing of the thermal stability due to the alginate crosslinking effect, particularly when $CaCl_2$ was used. The overall results showed that $CaCl_2$ is the most effective calcium source for alginate crosslinking, while calcium lactate lead to a more gradual release of the active principles.

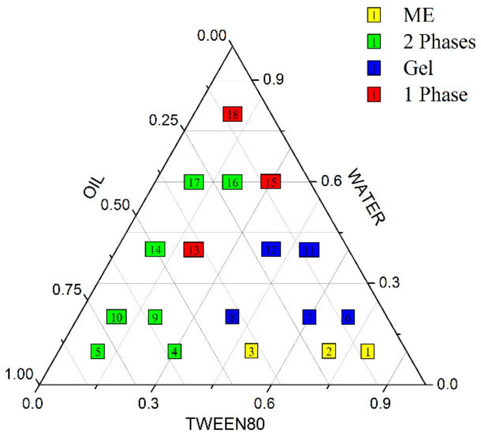
[P-IM36]

Emulsions preparation based on ternary phase diagrams: comparative study using two oils (miglyol and sweet almond) with two distinct surfactants (Tween 80 and Saponin)

T.L.B. Schreiner[1,2,3], M.M. Dias[3], S.P.Pinho[1,2,*], M.F. Barreiro[1,2,*]*

[1]CIMO, Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança; [2]LSRE-LCM, Polytechnic Institute of Bragança, Campus Santa Apolonia Ap 1134, 5301-857 Bragança, Portugal, Portugal, [3]LSRE-LCM, Department of Chemical Engineering, Faculty of Engineering of University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.

* pinho@ipb.pt , barreiro@ipb.pt

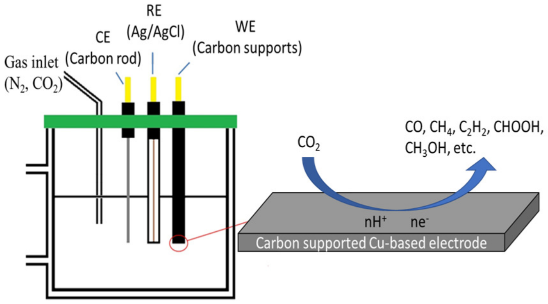


An emulsion is a colloidal dispersion composed by a mixture of two immiscible liquids, being one the dispersed phase, as droplets, and the other one the continuous phase. In this work, a comparative study comprising the surfactants Tween 80 (synthetic surfactant) and Saponin (natural surfactant) and the oils Miglyol 812 and Sweet Almond was performed. The development of emulsions based on ternary phase diagrams showed that different phases can be formed giving rise to different formulations: microemulsions, gels, and mixtures with 1, 2 and 3 phases. The application of the HPH technique produced stable nanoemulsions with narrow distributions. Considering Tween 80, and comparing the two oils, Miglyol 812 gave rise to emulsions with lower particle size (0.023µm), comparatively to Sweet Almond Oil (1.009µm). This difference can be related with the oil viscosity, which is lower for Miglyol 812. Comparing the two surfactants, natural Saponin was very effective in the o/w composition range.

[P-IM37]

The effect of treating the carbon supports on the copper electrocatalytic activity towards the electroreduction of CO_2

N.M. Pereira[1], *C. Mateos-Pedrero*[1], *A. Mendes*[1,*]
[1] LEPABE – Laboratory for Process Engineering, Environment, Biotechnology and Energy Institution*, Engineering Faculty of University of Porto – Department of Chemical Engineering, Rua Dr. Roberto Frias, s/n, Porto, Portugal*
* *mendes@fe.up.pt*

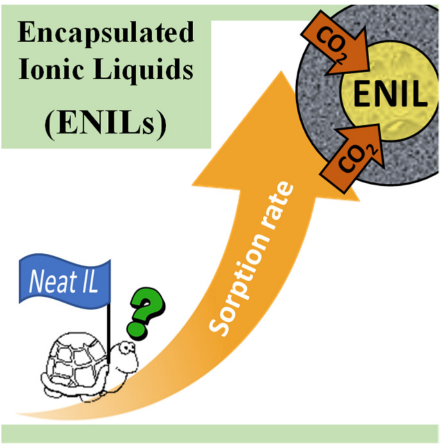


The carbon support effect on the electrocatalytic reduction of CO_2 was studied using nanostructured carbon materials, which were treated using different oxidizing routes or functionalized with heteroatoms. The effects of the pretreatment on the carbon support materials was evaluated by N_2 adsorption and X-ray photoelectron spectroscopy (XPS). It was found that the chemical surface properties and surface area were significantly modified after treating the carbon supports. The electrocatalytic activity was measured using linear sweep voltammetry, which showed that the introduction of oxygen or the functionalization with heteroatoms have a major impact on the electroreduction rate of CO_2.

[P-IM38]

From Kinetics to Equilibrium Control in CO_2 capture columns using Encapsulated Ionic Liquids (ENILs)

*C. Moya**[1], *R. Santiago*[1], *J. Lemus*[1], *D. Moreno*[1], *J. Palomar*[1]
[1] *Sección Ingeniería Química. Universidad Autónoma de Madrid. 28049 Madrid. Spain*
* *cristian.moya@uam.es*

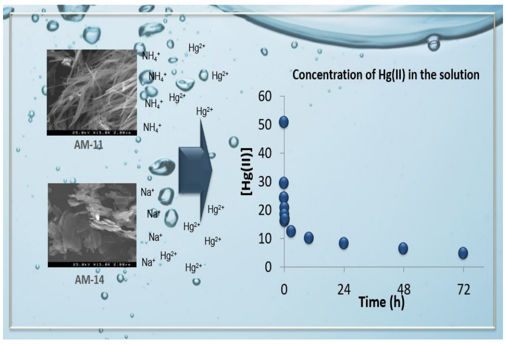


A novel approach based on Encapsulated Ionic Liquids (ENILs) is proposed for overcoming the mass transfer constraints in CO_2 physical absorption by ILs. Experimental gravimetric analyses with the 4 ILs selected (EmimTCM, BmimTCM, BmimDCN, and $BmimOcSO_4$) were carried out. Following, ENIL materials were prepared by encapsulation of ILs in hollow carbon sub-microcapsules with a porous shell. The experimental gravimetric analysis evidenced that the ILs maintain their CO_2 absorption capacity after encapsulation, whereas the absorption rate is ca. 50 times higher for ENILs than neat ILs. ENIL tests in fixed bed operation at different operating conditions yielded bed utilization values dependent on the CO_2 solubility in the ENIL, while equivalent mass transfer zone lengths were obtained for all the materials. The results demonstrate the fast CO_2 mass transfer rates in ENILs -related to the high contact area provided- allows overcoming the mass transfer limitations controlling the CO_2 rate of physical absorption by ILs.

[P-IM39]

New promising microporous niobium and vanadium silicates for mercury removal from aqueous solutions

E. Fabre[1,2*]*, A. Rocha*[1,2]*, C.B. Lopes*[1]*, C. Vale*[3]*, C.M. Silva*[1]*, E. Pereira*[2]
[1] *CICECO, Department of Chemistry, University of Aveiro, Aveiro, Portugal;* [2] *CESAM, Department of Chemistry, University of Aveiro, Aveiro, Portugal;* [3] *CIIMAR, University of Porto, Porto, Portugal.*
* *elainefabre@ua.pt*



Mercury is a hazardous toxic metal and its serious impacts to human health and environment make necessary its removal even at very low concentrations. In this work, two new microporous materials, AM-11 (niobium silicate) and AM-14 (vanadium silicate) have been tested for Hg(II) removal from aqueous solutions. Small doses of these solids (3.5-14.0 mg L^{-1}) have removed most of the metal in solution (81-99 %). Well known isotherms were applied for equilibrium study and the best fits have been obtained with Langmuir and Temkin equations, for AM-11 and AM-14, respectively. The ion exchange capacities obtained from Langmuir isotherm for AM-11 (161 mg g^{-1}) and AM-14 (304 mg g^{-1}) highlight the promising potential of these new sorbents for water treatment applications.

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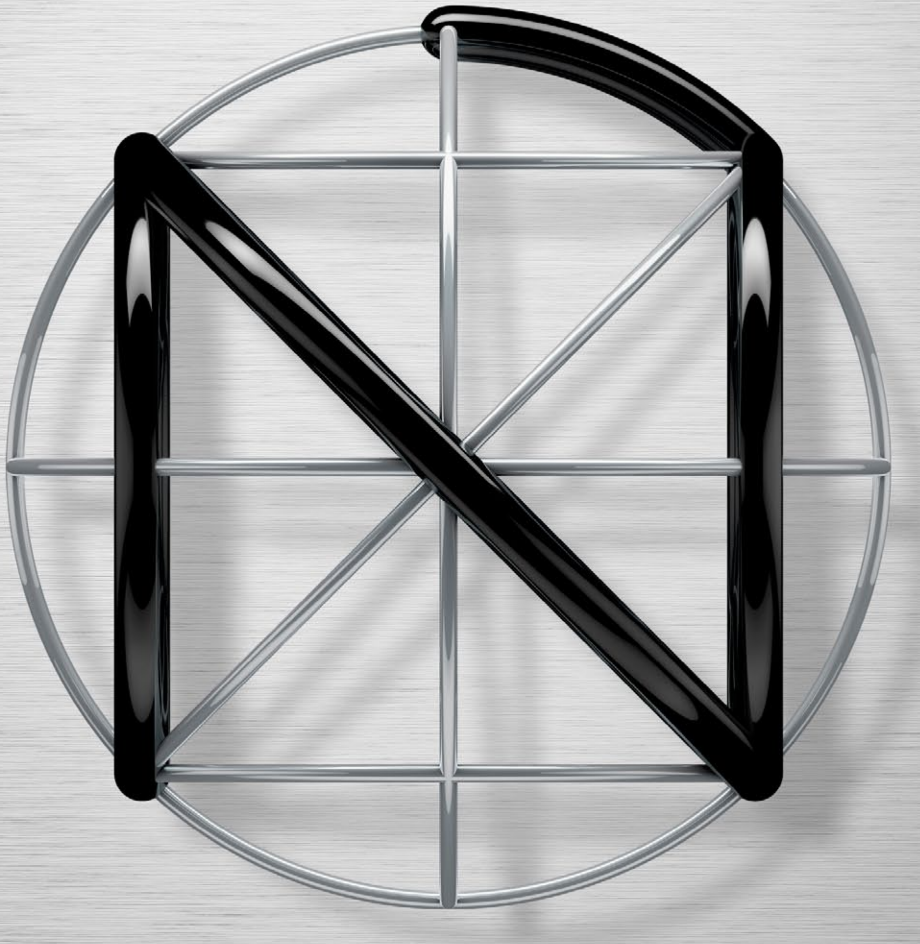

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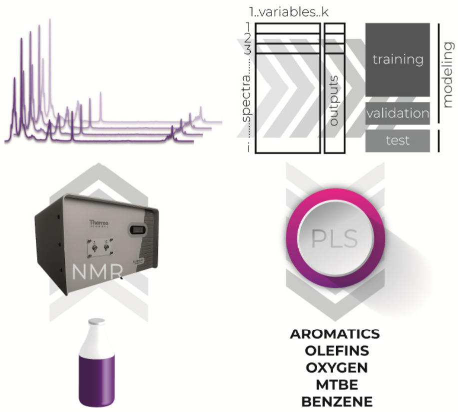
Poster Session

MODELING, SYNTHESIS AND INTEGRATION OF CHEMICAL PROCESSES

[P-MP01]

^{1}H NMR spectroscopy combined with partial least squares regression for predicting gasoline composition

A. L. Leal[1,2,3*], *J. C. Ribeiro*[2], *A. M. S. Silva*[1], *F. G. Martins*[3]
[1]*QNOPNA, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal;*
[2]*Petrogal, s. a., Refinaria de Matosinhos, Laboratório, Rua Belchior Robles, 4451-852 Leça da Palmeira, Portugal;*
[3]*LEPABE, Chemical Engineering Department, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.*
** eq10048@gmail.com*

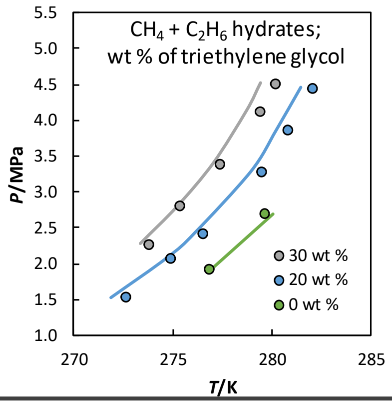


Proton nuclear magnetic resonance spectroscopy allows the expeditious and accurate quantitative evaluation of gasoline composition. Partial least squares regression models were developed using training and validation sets of a database containing 212 gasoline samples spectra and the respective composition values, obtained by the reference method. The multivariate data analysis was performed for five different compounds/groups: aromatic, olefin, benzene, methyl *tert*-butyl ether and oxygen content. The results show that the models can predict gasoline composition with high accuracy, presenting determination coefficients above 0.90 for the test data set. The statistical parameters obtained in terms of standard prediction errors are, in most cases, lower than the reproducibility values of the reference method. These facts indicate that this methodology is a powerful alternative for predicting gasoline composition.

[P-MP02]

Modeling clathrate hydrate formation/inhibition using a modified CPA EoS

A.M. Palma[1], *A.J. Queimada*[2,*], *J.A.P. Coutinho*[1]
[1] *CICECO – Universidade de Aveiro, Campus de Santiago 3810-193 Aveiro, Portugal;* [2] *KBC Advanced Technologies Limited (A Yokogawa Company), 42-50 Hersham Road, Walton-on-Thames, Surrey, United Kingdom;*
** aqueimada@kbcat.com*



A modified Cubic Plus Association (CPA) EoS is applied here in combination with the van der Waals-Platteeuw (vdWP) model, enabling the simultaneous description of liquid, gas and hydrate phases. Single and mixed guest hydrate formers are analyzed in the presence of the most common hydrate inhibitors. CPA is the most successful model for hydrate phase formation and inhibition in the Oil and Gas industry. However, without using a large number of binary interaction parameters between water and the inhibitor it is usually not possible to describe simultaneously their SLE and VLE, while accurately describing the hydrate phase. The present model was applied using a maximum of two binary interaction parameters between water and the hydrate inhibitors. This in turn increased the predictive capacity of the approach, while being able, in most cases, to describe freezing point depressions, VLE and hydrate dissociation

[P-MP03]

Heat exchanger network retrofit of an aromatics plant process unit using a hybrid methodology

V.E. Araújo[1,2,3], F.P. Bernardo[2], C.M. Reis[1], F.G. Martins[3]*
[1]Galp energia, Refinaria de Matosinhos, 4451-852 Leça da Palmeira, Portugal; [2] GEPSI-PSE Group, CIEPQPF, Department of Chemical Engineering, University of Coimbra, 3030-790 Coimbra, Portugal; [3] LEPABE - Laboratory for Process Engineering, Environment, Biotechnology and Energy, University of Porto, Rua Dr. Roberto Frias, 4200-464 Porto, Portugal.
** vanessa_araujo@live.com.pt*

HYBRID METHODOLOGY

1st Stage: Pinch Analysis
- Composite Curves for an HRAT;
- Grid Diagram of actual HEN to locate inneficient zones of of heat integration;

Input Data

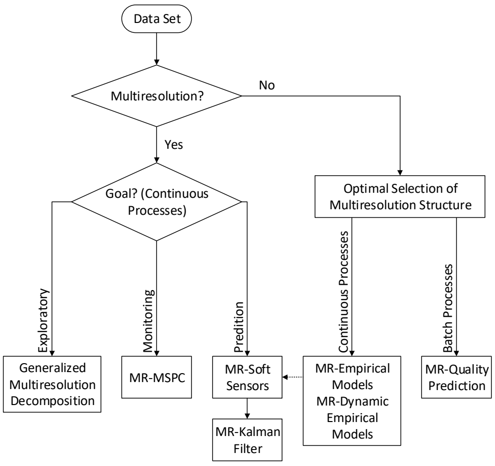
2st Stage: Retrofit to attain maximum heat recovery with minimum investment
- Minimum number of units (MILP model);
- Optimal HEN configuration and streams branches parameters (NLP/MINLP models).

Aromatics plants of petroleum refineries are energy-intensive consumers. The Pre-Distillation Unit of Matosinhos Refinery`s Aromatics Plant is here subjected to a heat integration and optimization study, in order to maximize heat transfer efficiency and thus reduce operating costs. For this purpose, a hybrid methodology, combining pinch analysis and mathematical programming tools, is developed for the retrofit of heat exchanger networks with minimum investment cost, and respecting minimum energy requirements. These are estimated through the construction of composite curves provided by pinch analysis. A grid diagram is used to represent the current network and to locate inefficient zones of heat integration. The inefficient zones are then removed using mathematical programming tools through the implementation of the sequential methodology. First results are very encouraging, with an estimated payback period of about 1 year and 2 months.

[P-MP04]

Advanced multi-granularity analytics for industry 4.0

M. S. Reis[1,] T.J. Rato*
[1] CIEPQPF – Dept. Chemical Engineering, University of Coimbra, Pólo II, Rua Sílvio Lima, 3030-790 Coimbra, Portugal
**marco@eq.uc.pt.*

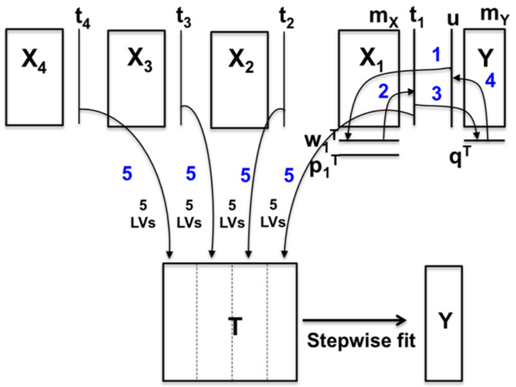


Data collected from industry present a variety of data structures, reflecting the evolution of industrial processes, measurement systems and IT infrastructures. Data analytics platforms must adapt to this new reality and keep the pace of its evolution in order to continue providing effective solutions to practitioners for dealing with the large data resources now available. In this context, one prevalent feature of industrial data has been largely overlooked: the existence of data with multiple granularities. The multi-granularity nature of data is directly connected to their aggregation in the time domain, an aspect that induces inner dependencies that current frameworks cannot address in a consistent and rigorous way. Furthermore, multi-granularity data have been often mistakenly treated as multirate data, where in fact the meaning of the observations is completely different. This results in suboptimal methodologies and outcomes not reaching the desired goals. In this paper, we highlight such differences and discuss current multi-granularity frameworks for effectively handling industrial data sets.

[P-MP05]

Structured multiblock approaches for high-dimensional predictive modeling

M.S. Reis[1,*]
[1] CIEPQPF – Dept. Chemical Engineering, University of Coimbra, Pólo II, Rua Sílvio Lima, 3030-790 Coimbra, Portugal
*marco@eq.uc.pt.

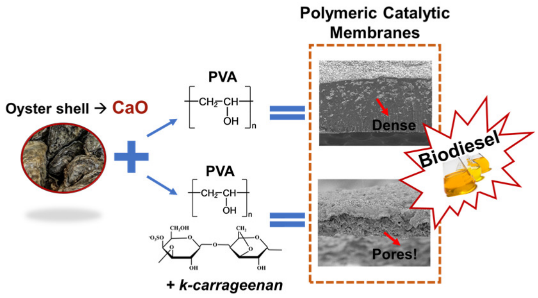


Current predictive approaches are strongly focused on optimizing accuracy metrics, leaving little room to incorporate *a priori* knowledge about the processes under analysis and relegating to a secondary concern the interpretation of results. However, there is often information available regarding the structure of the processes, which could be used in benefit of the analysis and to enhance the interpretation of results. The importance of this issue is not new and has motivated the development of multiblock approaches for improving interpretation while maintaining the quality of predictions. In this communication, two classes of multiblock frameworks are addressed. One class is based on the existence of a priori knowledge for building the blocks of variables, while methods from the second class are able to infer the system structure in a data-driven way. The introduction of such block structures constraint the predictive spaces for the sake of enabling interpretable elements in the final model. We show that such constraints do not usually compromise the methods' performances when compared to their unconstrained counterparts, and sometimes even led to improvements in prediction ability, due to the use of more parsimonious and robust models.

[P-MP07]

Polymeric catalytic membranes for biodiesel production – Effect of the addition of *k*-carrageenan in PVA membranes

R. Risso*, M. Ventura, C. Duarte, I. Fonseca, J. Vital
NOVA University of Lisbon / Faculty of Sciences and Technology, Quinta da Torre, Caparica, Portugal.
* r.risso@campus.fct.unl.pt

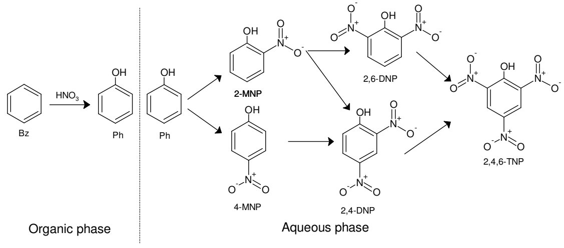


Composite catalytic membranes were prepared with poly(vinyl alcohol) (PVA) and *k*-carrageenan (KCA) blends and cross-linked with hexamethylene diisocyanate (HDI). The phase inversion process is performed after crosslinking. CaO derived from oyster shells was synthesised, treated with hydration cycles and employed as catalyst dispersed in the polymeric matrix. The catalytic membranes were used in the biodiesel synthesis by transesterification of soybean oil. Swelling degree, SEM and elemental analyses were used to characterise the membranes. The catalyst leaching was also determined. The characterisation results indicate that the phase inversion process partially removes the KCA, affecting the membrane structure with pore formation. The results show that the swelling is higher the higher the membrane porosity, and the presence of KCA minimises the catalyst leaching.

[P-MP08]

(Nitro)phenols reactivity in mixed acid benzene nitration

D. Afonso[1,2,3*], *A. Ribeiro*[1], *P. Araújo*[1], *J. Vital*[2], *L.M. Madeira*[3]
[1]*Bondalti CHEMICALS, S.A. Quinta da Indústria, Rua do Amoníaco Português, nº 10 Beduído, 3860-680 Estarreja, Portugal;*
[2]*REQUIMTE/CQFB, Faculdade de Ciências e Tecnologia, Universidade Nova de, Lisboa, 2829-516 Caparica, Portugal;*
[3]*LEPABE, Departamento de Engenharia Química, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal.*
** diogo.afonso@bondalti.com.*



Graphical Abstract. Nitrophenols interconversion scheme.

Phenol-benzene mixtures were nitrated in mixed acid systems, employing smooth conditions for enabling both phenol detection in the reaction medium and the construction of a simple kinetic model for this highly reactive species nitration while supporting the mechanism of phenol as the nitrophenols precursor. Benzene (phenol-free) nitration was also carried out, in reaction conditions similar to the ones employed in the industrial production of mononitrobenzene, aiming the detection of all reaction by-products formed by phenol nitration, while also evidencing its high reactivity. The effect of some operating conditions, namely the reaction temperature, sulfuric acid concentration and mixed acid composition, were evaluated, which allowed verifying that upon phenol formation, nitrophenols are formed by consecutive reactions, i.e., mononitrophenols are nitrated into dinitrophenols that are the

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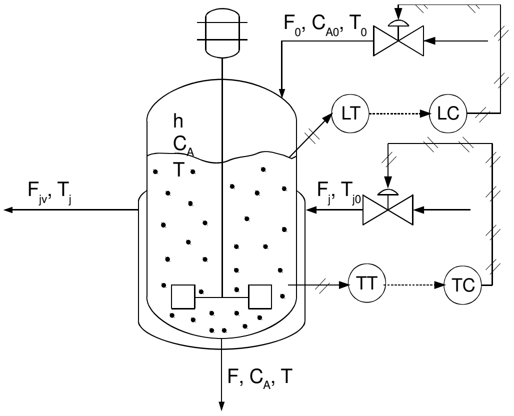
[P-MP09]

Simulation, monitoring and diagnosis of faults and equipment degradation in chemical processes

J. Sansana[1] , *M. Reis*[1,*]
[1] *CIEPQPF - Department of Chemical Engineering, University of Coimbra, Rua Sílvio Lima, Polo II, 3030-790 Coimbra, Portugal,*
**marco@eq.uc.pt*

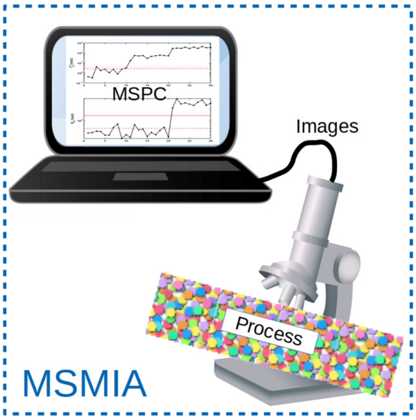


Fault detection and diagnosis is a mature field of Process Systems Engineering, with many contributions being proposed throughout more than 40 years of active research. The proposed methodologies address mostly abrupt faults in the process, sensors or actuators. However, monitoring equipment degradation, has not received much attentions, despite its critical importance for industrial companies. Therefore, in this work, a simulator was developed that emulates a process containing the fundamental features of real industrial units and several abrupt faults were simulated, as well as different equipment degradation phenomena. Multivariate and multiscale methodologies were then applied for detecting and analyzing all these different events occurring at different time scales. Results reveal that it is possible to diagnose equipment degradation, and point to some limitations of existing methods for abrupt fault diagnosis that need to be addressed in the future.

[P-MP10]

Image-based process monitoring using multiscale and multivariate image analysis: A pilot scale implementation study and results

E. Strelet[1,] M. Reis[1,*]
[1] CIEPQPF - Department of Chemical Engineering, University of Coimbra, Rua Sílvio Lima, Polo II, 3030-790 Coimbra, Portugal; *marco@eq.uc.pt.

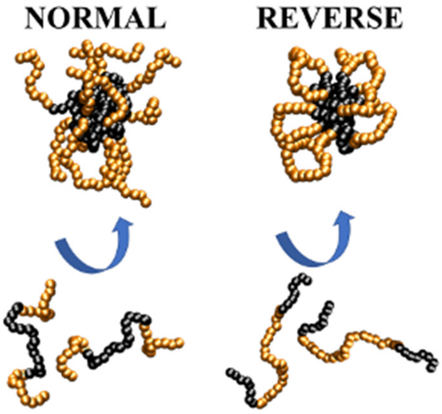


With this work, we establish the validity and usefulness of the Multiscale and Multivariate Image Analysis (MSMIA) approach for image-based process monitoring, proposed by M. Reis [1], by applying it online in a pilot scale hardware system. The MSMIA methodology combines wavelet texture analysis and multivariate image analysis, for detecting both abnormal changes in texture and color. The approach was implemented in a pilot scale system and applied to several controlled testing scenarios. The scenarios include normal operation conditions (NOC) and faults of different types and magnitudes. Therefore, it was possible to assess the monitoring potential of the proposed methodology to detect abnormal process conditions under various types of faulty conditions related to the size, shape and color of the image attributes. Results confirm the sensitivity of MSMIA to perform image-based fault detection when applied on real images.

[P-MP11]

A coarse-grain computer simulation approach of triblock copolymers

G. Pérez-Sánchez[1,*], F.A. Vicente[1], N. Schaeffer[1], S.P.M. Ventura[1] J.A.P. Coutinho[1]
[1] CICECO, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal.
* gperez@ua.pt

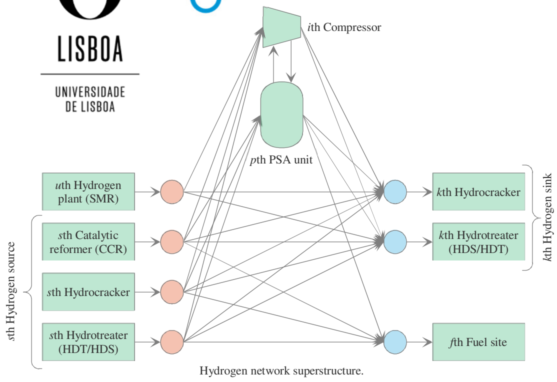


The advent of the transferable MARTINI coarse-grain (CG) model boosted the applicability of computer simulations to study the self-assembly of complex systems. However, despite a great paperwork developed in the recent years, a general model for Triblock copolymers (TBC) is still lacking. In this study, the CG model was developed to reproduce, by computer simulations, the essential physico-chemical characteristics of TBC in aqueous solutions. For this purpose, an archetypical normal and reverse TBC with different amphiphilic character were chosen. Our CG approach was validated by comparing selected computer simulation results with experiments carried in our laboratory and literature data.

[P-MP12]

Galp's Sines Refinery Hydrogen Network Optimisation

J.P. Marques[1], *H.A. Matos*[1,*], *N.M.C. Oliveira*[2], *C.P. Nunes*[1], *A. Guerreiro*[3], *M.Prego*[3]
[1] *Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal;* [2] *Universidade de Coimbra, R. Sílvio Lima - Pólo II, 3030-790 Coimbra, Portugal;* [3] *Galp SGPS S.A., Rua Tomás Fonseca - Edifício Galp, 1600-211 Lisboa, Portugal;*
* *henrimatos@tecnico.ulisboa.pt*



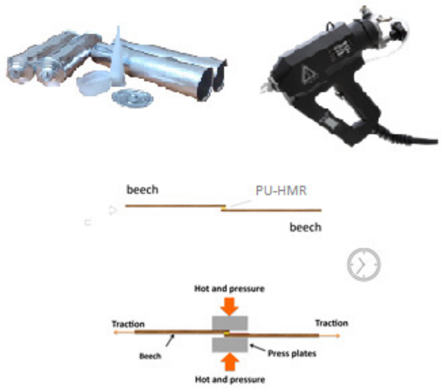
Hydrogen network superstructure.

The grassroots and retrofit design of hydrogen distribution systems has been actively investigated since the 2000's either using mathematical programming or simply relying on insight-based methods. This paper intends to present the optimisation model that has been developed so far for the retrofit design of Galp's Sines refinery hydrogen network. The retrofit design model depicted here represents only one part of a complex optimisation framework, which includes data conditioning, reconciliation, and Pinch Analysis. The objective is to find the optimal flowsheet configuration that leads to the lowest operational expenses with minimal capital expenditure involved such as new connections, PSA units, and compressors and minimal configuration complexity. For the current flowsheet configuration, a total annual cost saving of approximately 3,400 u.year^{-1} can be easily obtained just by redirecting some of the off-gas streams that are being disposed of to the fuel gas system to a PSA unit. This solution requires, however, the revamping of the existing PSA unit since the former has already reached its full capacity. A payback period of 1.1 years is expected after the proposed solutions are implemented. This project was carried out as part of a joint venture between Galp, IST, and the U. Coimbra.

[P-MP13]

Synthesis and characterization of reactive polyurethane hotmelt adhesives

J. Martins[2,3], *I.C.S. Cardoso* [1], *C.S.V.G. Esteves*[4], *M.M.S.M. Bastos*[2], *J.C.F. Fernandes*[4], *N. Pinho*[5], *M.F. Barreiro*[6], *F.D. Magalhães*[2], *L.H. Carvalho*[2,3*]
[1] *ARCP – Associação Rede de Competência em Polímeros, UPTEC-Pólo Inovação, Rua Júlio de Matos 828, 4200-355, Portugal;* [2] *LEPABE, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;* [3] *DEMad - Instituto Politécnico de Viseu, Campus Politécnico de Repeses 3504-510, Viseu, Portugal;* [4] *Lorcol, Avenida 1º De Maio, São João Da Madeira, Aveiro, 3700, S. João da Madeira, Portugal;* [5] *Vicaima, Av. António Alberto de Almeida Pinheiro, 3730-135 Vale de Cambra;* [6] *CIMO – Centro de Investigação de Montanha and LSRE-LCM, Instituto Politécnico de Bragança, Campus de Santa Apolónia Ap. 1134, 5301-857-Bragança.*
**lhcarvalho@estgv.ipv.pt*



Synthesis of polyurethane materials was developed by Otto Bayer in 1937 and they became the most important organic polymers for technological applications. Polyurethane hot melt adhesives (PU-HMR) have attracted high attention and have been widely used, because of their features such as good green strength, excellent adhesion to multiple substrates and good resistance to heat [1]. These type of adhesives are prepared from polyester- and/or polyether-based polyols and diisocyanates. In this work, PU- HMR synthesis using different formulations was performed in order to evaluate the influence of the most important parameters on bonding performance and though their ability for edge banding in doors manufacture. Different polyols and isocyanates were tested. Adhesive characteristics such as the final viscosity, open time, wood bonding and thermal properties, were studied. The green strength, as well as the final cure were evaluated by ABES.

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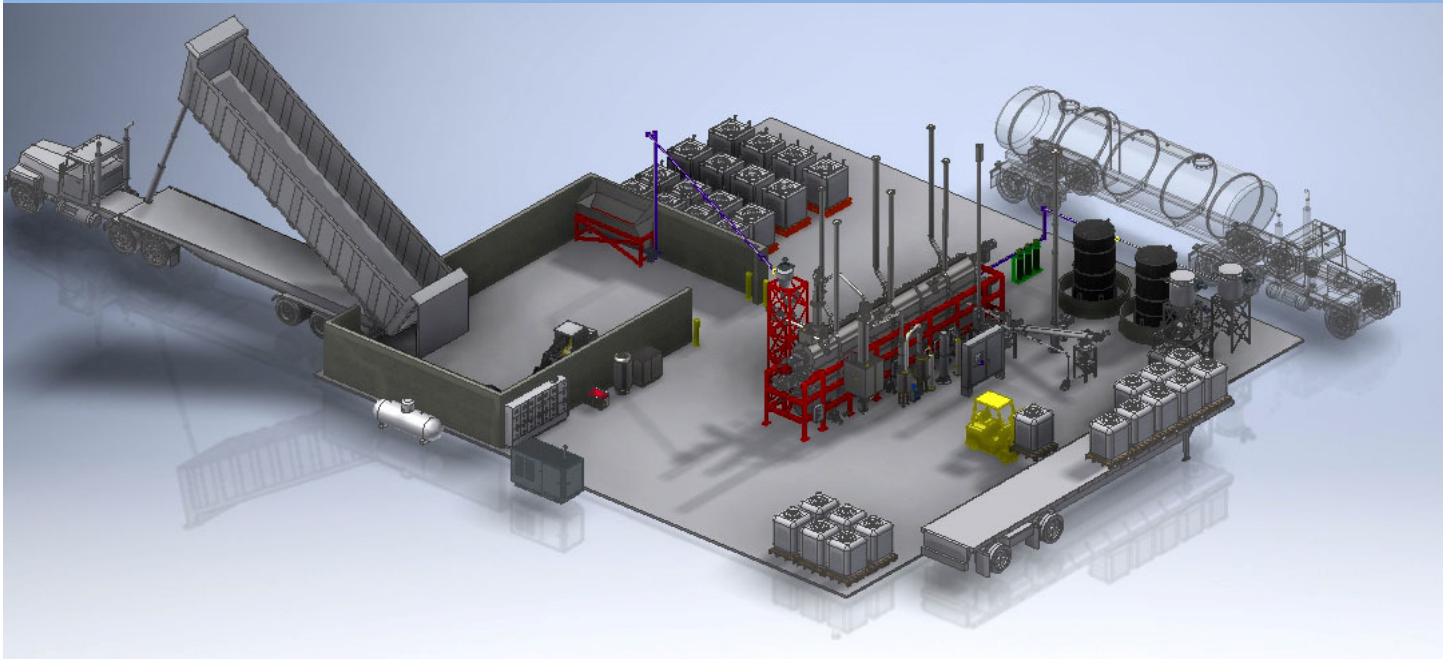
Company Overview



Contact Information

Germano Carreira, MBA
Chief Executive Officer
BB&G AWES
Alternative Worldwide Enviromental Solutions
germano@bbgenv.com

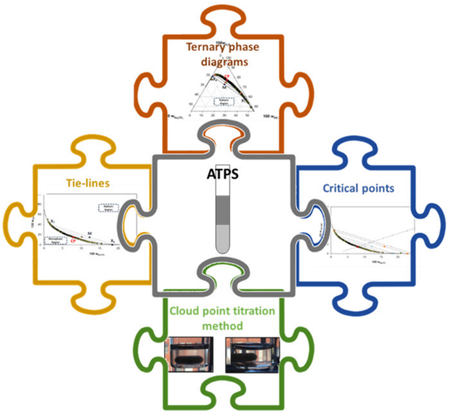
Poster Session

MULTISCALE AND MULTIDISCIPLINARY ENGINEERING EDUCATION

[P-ME01]

A simple laboratory approach for the determination and characterization of ternary phase diagrams for Chemical Engineering undergraduate students

E.V. Capela[1], J.H.P.M. Santos[1], I. Boal-Palheiros[1], J.A.P. Coutinho[1], S.P.M. Ventura[1], M.G. Freire[1,*]
[1] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.
* maragfreire@ua.pt

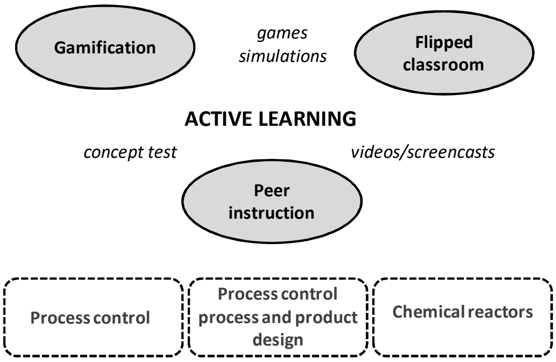


In this work, a simple experimental protocol to determine liquid-liquid phase diagrams of aqueous two-phase systems (ATPS) on a Chemical Engineering course is described. To this end, the liquid-liquid phase diagrams composed of water, PEG (200, 400, 600 and 1000 $g \cdot mol^{-1}$) and sodium carbonate (Na_2CO_3) must be determined through the cloud-point titration method at the laboratory room temperature. Throughout this laboratory set of experiments, the liquid-liquid ternary phase diagrams, tie-lines, tie-line lengths and critical points of ATPS were determined. This novel educational approach could be potentially used to teach and help understanding 3-component liquid-liquid equilibrium as well as the formation of biphasic systems to undergraduate students, without requiring the use of volatile organic solvents.

[P-ME02]

Promoting an active learning in subjects of the Chemical Engineering degree

E. J. González*, I. Díaz, M. Rodríguez, M. González-Miquel
Departamento de Ingeniería Química Industrial y del medioambiente, Universidad Politécnica de Madrid, C/José Gutiérrez Abascal, 2, E-28006 Madrid, Spain.
* ej.gonzalez@upm.es

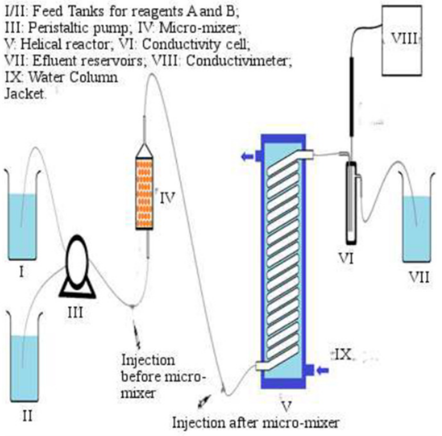


The purpose of this work is to promote an active learning based on the joint use of several methodologies (flipped classroom, peer instruction or gamification) in several subjects of the Chemical Engineering Degree at the Technical University of Madrid. Specifically, this approach has already been implemented in Process Control (4th course) and will also be applied in Process and product design (4th course) and Chemical Reactors (3rd course) during the next academic year. In order to implement the mentioned methods, the following material has been developed: screencasts, concept tests, trivia contest and simulations besides the traditional material (slides and text).The results obtained in Process control subject after the implementation of this methodology for the first time show increasing student motivation, higher participation in class and better results (marks) in the subject. The same results are expected for the other two subjects.

[P-ME03]

Exploring the non-ideal behavior of coiled and straight tubular reactors

N.V. Gama, F.A. Da Silva, I. Portugal*
Department of Chemistry & CICECO – Aveiro Institute of Materials, University of Aveiro / Campus Universitário de Santiago, 3810-193 Aveiro, Portugal
** fsilva@ua.pt*

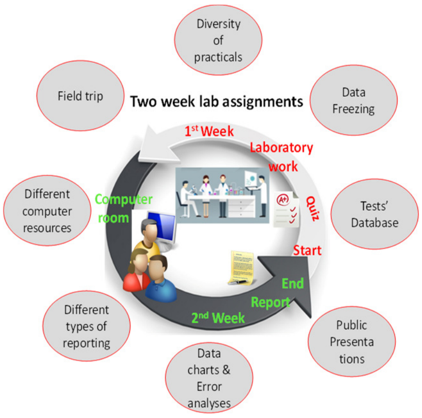


Flow characterization in chemical reactors is a challenging and important topic in chemical engineering education. This work describes a simple and inexpensive experimental set-up for determining residence time distribution (RTD) curves in tubular reactors, using a conductivity cell to measure the outlet concentration of a pulse injection of an inert tracer. The experimental results are compared with different model alternatives (e.g. laminar flow, cascade of n-CSTR, axial dispersion) and used to evaluate the characteristic parameter(s). In a second stage, the saponification of ethyl acetate is performed in the tubular reactors to evaluate steady state conversion. The results are compared with predicted conversions obtained with the total segregation model and the suggested RTD model alternatives. The experimental procedure and calculations were performed by several students at University of Aveiro and proved to be very useful to grasp the underlying concepts.

[P-ME04]

Pushing the dynamics and the outputs of laboratory courses

A.B. Timmons, F.A. Da Silva*
CICECO, Chemistry Department, University of Aveiro / Campus Universitário de Santiago, Aveiro, Portugal.
*anabarros@ua.pt

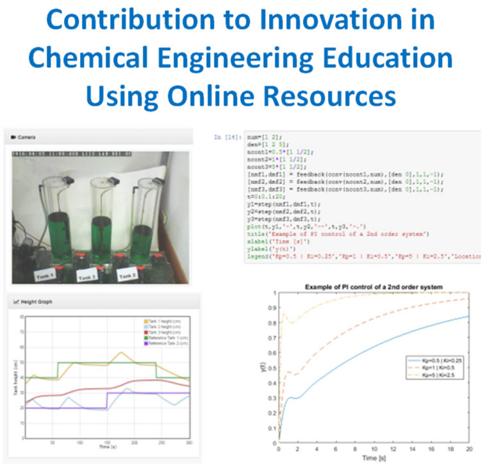


Experimental courses contribute to the development of practical skills as well as a series of soft skills. Furthermore these courses are also useful to demonstrate the relevance of the fundamental courses taught previously and help the students to go through a self-evaluation process of the command they have of theory. When large numbers are involved, i.e. 2 or 3 classes with circa 15 students, continuous supervision can be challenging task, especially if the flow and dynamics of practical work are to be kept throughout the entire semester. In this work we present and discuss the set of activities that are being used in 4th year Chemical Engineering laboratory classes in order to push the dynamics and the outputs in these courses.

[P-ME05]

Contribution to Innovation in Chemical Engineering Education Using Online Resources

A. Cardoso[1,], M. G. Rasteiro[2]*
*[1] CISUC, Dep. of Informatics Engineering, Pólo II da UC, Coimbra, Portugal; [2] Dep. of Chemical Engineering, Pólo II da UC, Coimbra, Portugal; *alberto@dei.uc.pt.*



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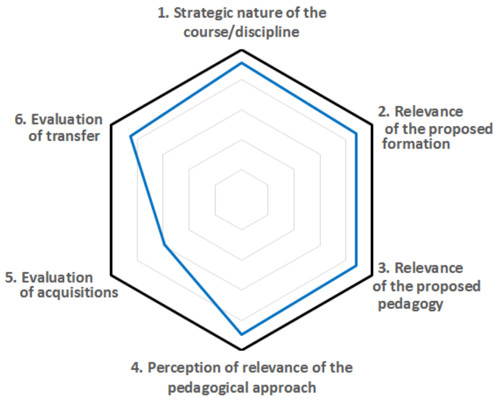
ncont2=1*[1 1/2];
ncont3=5*[1 1/2];
[nmf1,dmf1] = feedback(conv(ncont1,num),[den 0],1,1,-1);
[nmf2,dmf2] = feedback(conv(ncont2,num),[den 0],1,1,-1);
[nmf3,dmf3] = feedback(conv(ncont3,num),[den 0],1,1,-1);
t=0:0.1:20;
y1=step(nmf1,dmf1,t);
y2=step(nmf2,dmf2,t);
y3=step(nmf3,dmf3,t);
plot(t,y1,'-',t,y2,'--',t,y3,'-.')
title('Example of PI control of a 2nd order system')
xlabel('Time [s]')
ylabel('y(t)')
legend('Kp=0.5 | Ki=0.25','Kp=1 | Ki=0.5','Kp=5 | Ki=2.5','Locatio
```

The improvement of the teaching and learning activities, namely in Engineering education, should be a permanent concern of all involved actors and the existence of multiple tools and platforms to develop and provide online resources should be considered as an additional motivation to develop and implement innovative processes and materials. By providing materials and experiments online, students have the ability to use and access them without severe scheduling restrictions. Using Jupyter Notebook, teachers have a programming environment to develop and share educational materials through the web, combining different types of resources, such as text, images and code, into a single document. This article aims to contribute to innovation in Chemical Engineering education by presenting some examples of online resources supported by online experimentation and the Jupyter Notebook environment, which can be used to increase teacher productivity and enhance the students learning process.

[P-ME06]

Developing a framework for assessing the teaching effectiveness in Chemical Engineering education

C.V. Miguel[1], C. Moreira[1], M.A. Alves[1], J.M. Campos[1], J. Glassey[2], E. Schaer[3], N. Kockmann[4], A.P. Kujundziski[5], M. Polakovic[6], L.M. Madeira[1,]*
[1] Faculty of Engineering of University of Porto, Rua Dr. Roberto Frias, Porto, Portugal; [2] Newcastle University, Newcastle upon Tyne, United Kingdom. [3] ENSIC-LRGP, UL Nancy, France; [4] TU Dortmund University, Germany; [5] International Balkan University, Skopje, R. Macedonia; [6] Slovak Technical University, Bratislava, Slovakia.
*mmadeira@fe.up.pt

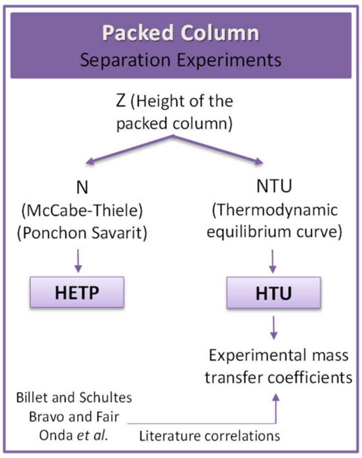


Evaluating the effectiveness of teaching and learning of core knowledge outcomes and professional skills is a highly challenging task that has not yet been satisfactorily addressed up to this date at higher education level. The iTeach European project consortium developed a framework for assessing the effectiveness of various pedagogical methodologies in chemical engineering education, in particular those aimed at promoting important core competencies related to employability, in a range of geographical and educational contexts. The framework was tested on a range of subject areas from various branches of engineering, and other areas. The results of this broader testing encompassed a much more diverse student body with varying educational experiences and a wider range of different teaching methodologies. The outcomes of this testing are highlighted and the benefits of such an objective approach to evaluating teaching effectiveness is discussed.

[P-ME07]

Design and efficiency assessment of a packed bed distillation column by HETP and HTU approaches

Andreia F. Silva[*], *A.A. Valente, F.A. Da Silva, C.M. Silva*
CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro, Portugal;
** andreiafreitas@ua.pt*



The knowledge of equilibrium and mass transfer phenomena is fundamental for the accurate modeling and design of rate-controlled separations. One may cite distillation, dehumidification, extraction and absorption carried out in packed columns, which are frequently covered by Chemical Engineering curricula. The present work focuses the efficiency of a packed column for the distillation of an ethanol-water mixture, where two approaches are compared: the Height Equivalent to a Theoretical Plate and the Height of a Transfer Unit. The column contains small glass spheres randomly dispersed, and two distinct internal flow rates are analyzed. The convective mass transfer coefficients are obtained from experimental data, and compared with estimations provided by various literature correlations, adequate for the type of packing and system under study. Bravo and Fair, and Billet and Schultes correlations were more suitable to calculate the mass transfer coefficients.

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